Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 05:18 pm GMT

PDB ID	:	1W20
Title	:	Structure of Neuraminidase from English duck subtype N6 complexed with 30 mM sialic acid (NANA, Neu5Ac), crystal soaked for 3 hours at 291 K
Authors	:	Rudino-Pinera, E.; Tunnah, P.; Crennell, S.J.; Webster, R.G.; Laver, W.G.; Garman, E.F.
Deposited on	:	2004-06-24
Resolution	:	2.08 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

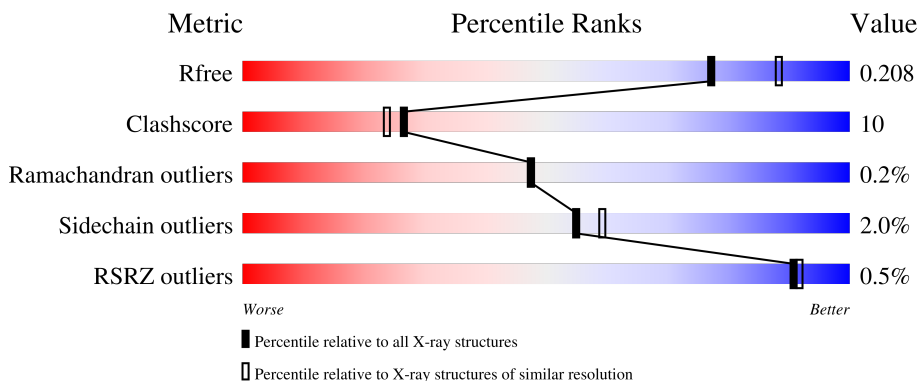|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
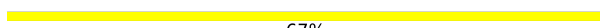
Metric	Percentile Ranks	Value
Rfree		0.208
Clashscore		10
Ramachandran outliers		0.2%
Sidechain outliers		2.0%
RSRZ outliers		0.5%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	389	86% 13% •
1	B	389	.% 86% 11% ••
1	C	389	.% 85% 13% •
1	D	389	85% 12% •

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Mol	Chain	Length	Quality of chain
2	E	2	100%
2	F	2	100%
2	H	2	100%
3	G	3	67%　　　　　33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	F	1	-	-	X	-
2	NAG	H	2	-	-	X	-
3	BMA	G	2	-	-	X	-
4	SIA	A	1478	-	-	-	X
4	SIA	C	3478	-	-	-	X
5	GOL	A	1479	-	X	-	-
5	GOL	B	2479	-	X	-	-
5	GOL	C	3479	-	X	-	-
5	GOL	D	4479	-	X	-	-
7	BMA	A	1484	-	-	X	-
8	MAN	A	1485	-	-	X	-
8	MAN	C	3486	-	-	-	X

2 Entry composition ⓘ

There are 10 unique types of molecules in this entry. The entry contains 14289 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NEURAMINIDASE SUBTYPE N6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	B	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	C	389	Total	C	N	O	S	0	0	0
			3008	1875	535	571	27			
1	D	389	Total	C	N	O	S	0	0	0
			3009	1875	535	572	27			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.
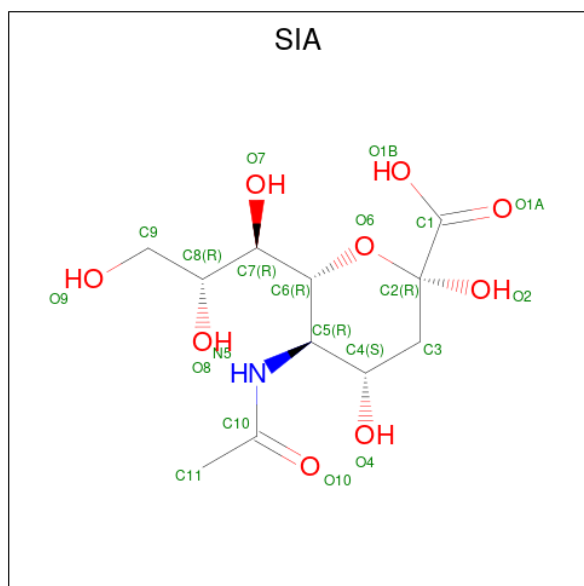

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	3	Total 36	C 20	N 1	O 15	0	0	0

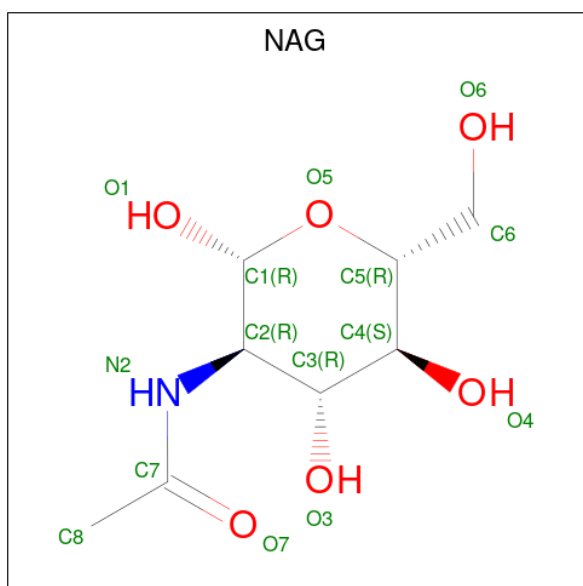- Molecule 4 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: $C_{11}H_{19}NO_9$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 21	C 11	N 1	O 9	0	0
4	A	1	Total 21	C 11	N 1	O 9	0	0
4	B	1	Total 21	C 11	N 1	O 9	0	0
4	B	1	Total 21	C 11	N 1	O 9	0	0
4	C	1	Total 21	C 11	N 1	O 9	0	0
4	C	1	Total 21	C 11	N 1	O 9	0	0
4	D	1	Total 21	C 11	N 1	O 9	0	0
4	D	1	Total 21	C 11	N 1	O 9	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

W O R L D W I D E
PDB
PROTEIN DATA BANK

GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 6	C 3	O 3	0	0
5	B	1	Total 6	C 3	O 3	0	0
5	C	1	Total 6	C 3	O 3	0	0
5	D	1	Total 6	C 3	O 3	0	0

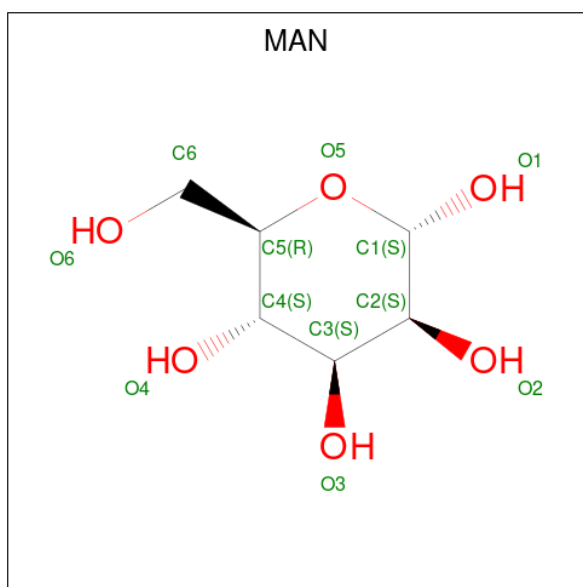- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 14	C 8	N 1	O 5	0	0
6	A	1	Total 14	C 8	N 1	O 5	0	0
6	B	1	Total 14	C 8	N 1	O 5	0	0
6	C	1	Total 14	C 8	N 1	O 5	0	0
6	D	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 7 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).
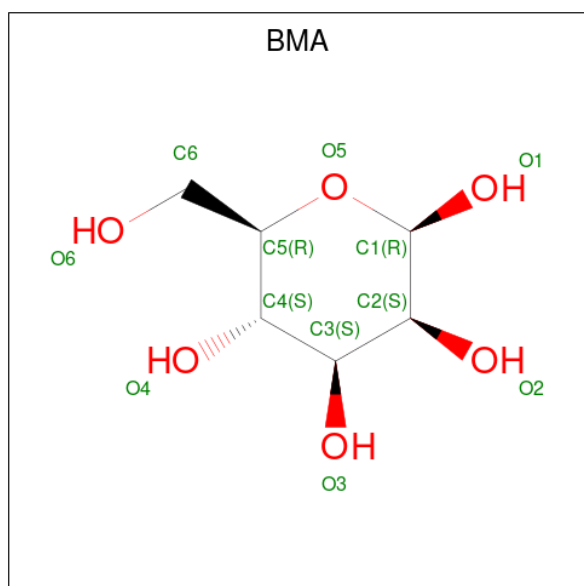
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 11	C 6	O 5	0	0
7	B	1	Total 11	C 6	O 5	0	0
7	C	1	Total 11	C 6	O 5	0	0

- Molecule 8 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).

MAN

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		
8	B	1	Total	C	O	0	0
			11	6	5		
8	B	1	Total	C	O	0	0
			11	6	5		
8	B	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Ca	0	0
			1	1		
9	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total 1	Ca 1	0	0
9	D	1	Total 1	Ca 1	0	0

- Molecule 10 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	430	Total 430	O 430	0	0
10	B	414	Total 414	O 414	0	0
10	C	427	Total 427	O 427	0	0
10	D	456	Total 456	O 456	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
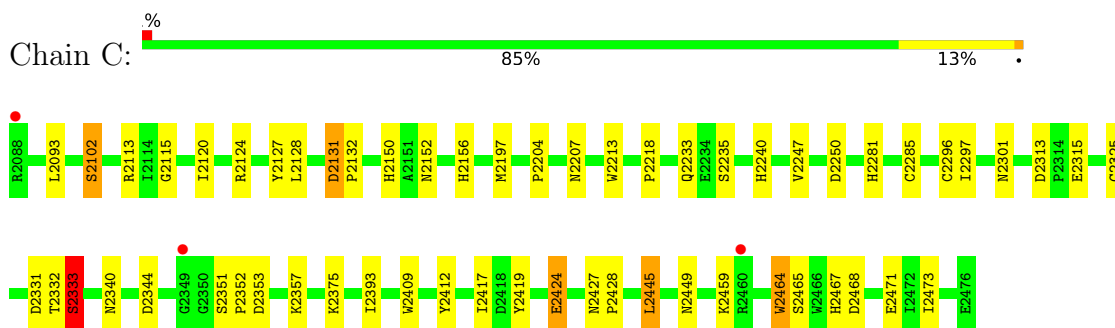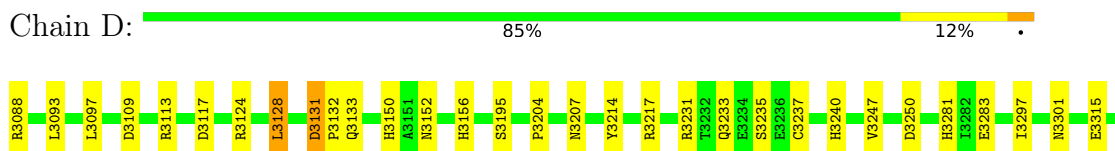
- Molecule 1: NEURAMINIDASE SUBTYPE N6
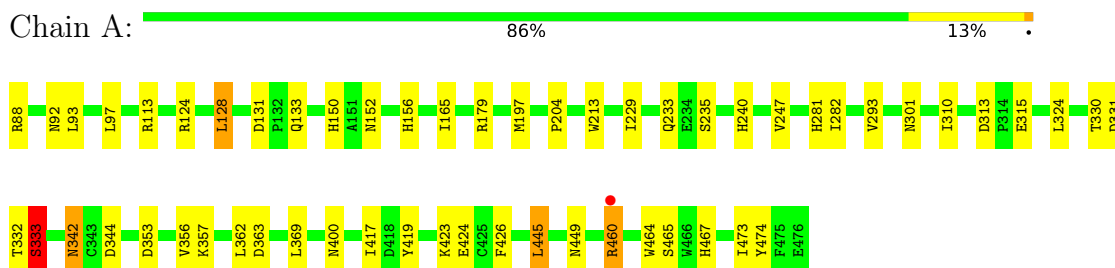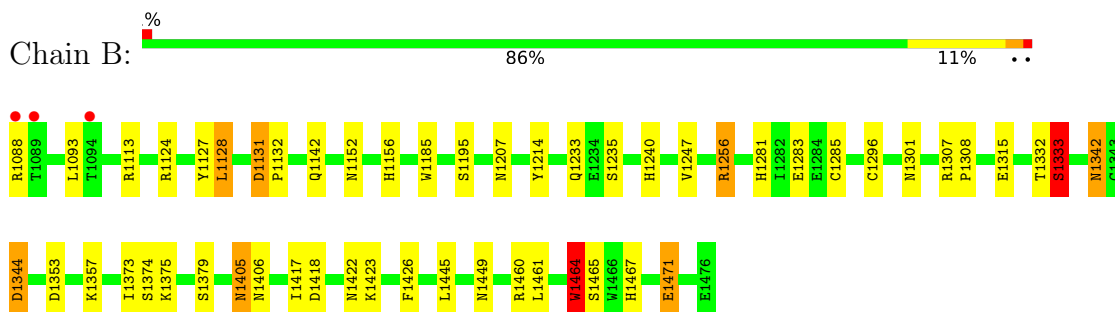
Chain A:

- Molecule 1: NEURAMINIDASE SUBTYPE N6

Chain B:

- Molecule 1: NEURAMINIDASE SUBTYPE N6

Chain C:

- Molecule 1: NEURAMINIDASE SUBTYPE N6

Chain D:

D3331 T3332 S3333 G3341 N3342 C3343 D3344 I3347 D3353 K3357 D3363 L3369 Y3381 V3386 A3389 D3392 S3395 E3424 P3428 L3445 N3449 R3460 L3461 W3464 D3468 G3469 A3470 E3471 I3472 I3473 E3476

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

100%

NAG1 NAG2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

100%

NAG1 NAG2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

100%

NAG1 NAG2

• Molecule 3: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

67% 33%

NAG1 BMA2 MAN3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.48Å 74.00Å 106.47Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	105.41 – 2.08 29.41 – 2.08	Depositor EDS
% Data completeness (in resolution range)	98.0 (105.41-2.08) 98.0 (29.41-2.08)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.150 , 0.195 0.161 , 0.208	Depositor DCC
R_{free} test set	4913 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	15.4	Xtriage
Anisotropy	1.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.2	EDS
L-test for twinning[2]	$< |L| >$ = 0.49, $< L^2 >$ = 0.32	Xtriage
Estimated twinning fraction	0.008 for -l,k,h 0.021 for -h,-k,l 0.015 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14289	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, NAG, BMA, CA, GOL, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	1.05	1/3083 (0.0%)	0.89	6/4185 (0.1%)
1	B	1.03	2/3083 (0.1%)	0.89	5/4185 (0.1%)
1	C	1.03	1/3083 (0.0%)	0.90	7/4185 (0.2%)
1	D	1.06	3/3084 (0.1%)	0.93	12/4185 (0.3%)
All	All	1.04	7/12333 (0.1%)	0.90	30/16740 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	3471	GLU	CD-OE2	6.73	1.33	1.25
1	B	1471	GLU	CD-OE2	6.62	1.32	1.25
1	C	2102	SER	CB-OG	-5.53	1.35	1.42
1	A	474	TYR	CE1-CZ	5.38	1.45	1.38
1	D	3217	ARG	CZ-NH2	5.09	1.39	1.33
1	D	3381	TYR	CD1-CE1	5.03	1.46	1.39
1	B	1464	TRP	CE3-CZ3	5.00	1.47	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3250	ASP	CB-CG-OD2	9.23	126.61	118.30
1	B	1344	ASP	CB-CG-OD2	7.47	125.02	118.30
1	B	1333	SER	N-CA-C	-7.36	91.13	111.00
1	C	2131	ASP	CB-CG-OD2	7.34	124.91	118.30
1	C	2333	SER	N-CA-C	-7.28	91.34	111.00
1	C	2250	ASP	CB-CG-OD2	7.14	124.72	118.30
1	D	3131	ASP	CB-CG-OD2	7.13	124.71	118.30
1	A	313	ASP	CB-CG-OD2	6.75	124.37	118.30
1	D	3468	ASP	CB-CG-OD2	6.65	124.28	118.30
1	D	3344	ASP	CB-CG-OD2	6.37	124.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	LEU	CA-CB-CG	6.33	129.87	115.30
1	A	333	SER	N-CA-C	-5.94	94.96	111.00
1	D	3333	SER	N-CA-C	-5.93	94.99	111.00
1	C	2313	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	2331	ASP	CB-CG-OD1	5.73	123.46	118.30
1	D	3353	ASP	CB-CG-OD2	5.73	123.46	118.30
1	C	2468	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	333	SER	CB-CA-C	5.56	120.67	110.10
1	C	2344	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	1131	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	1128	LEU	CB-CG-CD2	5.42	120.22	111.00
1	D	3128	LEU	CA-CB-CG	5.40	127.72	115.30
1	A	131	ASP	CB-CG-OD2	5.36	123.13	118.30
1	D	3128	LEU	CB-CG-CD2	5.34	120.07	111.00
1	D	3363	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	331	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	3109	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	3392	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	1418	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	3331	ASP	CB-CG-OD1	5.04	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3008	0	2888	50	0
1	B	3008	0	2888	54	0
1	C	3008	0	2888	51	0
1	D	3009	0	2888	55	0
2	E	28	0	25	10	0
2	F	28	0	26	10	0
2	H	28	0	26	10	0
3	G	36	0	33	10	0
4	A	42	0	36	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	42	0	36	4	0
4	C	42	0	36	4	0
4	D	42	0	36	4	0
5	A	6	0	4	2	0
5	B	6	0	4	1	0
5	C	6	0	4	1	0
5	D	6	0	4	1	0
6	A	28	0	26	5	0
6	B	14	0	13	3	0
6	C	14	0	13	3	0
6	D	14	0	13	3	0
7	A	11	0	10	6	0
7	B	11	0	10	3	0
7	C	11	0	10	4	0
8	A	33	0	30	6	0
8	B	33	0	30	2	0
8	C	44	0	40	10	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	C	1	0	0	0	0
9	D	1	0	0	0	0
10	A	430	0	0	5	0
10	B	414	0	0	13	0
10	C	427	0	0	8	0
10	D	456	0	0	7	0
All	All	14289	0	12017	247	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (247) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ASN:HD21	6:A:1480:NAG:C1	1.16	1.52
1:B:1152:ASN:HD21	6:B:2480:NAG:C1	1.35	1.38
1:C:2152:ASN:HD21	6:C:3481:NAG:C1	1.37	1.37
1:A:152:ASN:HD21	6:A:1481:NAG:C1	1.46	1.26
1:D:3152:ASN:HD21	6:D:4480:NAG:C1	1.62	1.12
1:B:1152:ASN:ND2	6:B:2480:NAG:C1	2.19	1.05
1:C:2152:ASN:ND2	6:C:3481:NAG:C1	2.19	1.05
1:A:152:ASN:ND2	6:A:1481:NAG:C1	2.22	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:2484:MAN:O6	8:B:2485:MAN:C1	2.09	1.00
1:D:3152:ASN:ND2	6:D:4480:NAG:C1	2.30	0.94
2:H:1:NAG:HO4	2:H:2:NAG:C1	1.62	0.94
1:B:1373:ILE:HB	10:B:2330:HOH:O	1.67	0.93
1:C:2093:LEU:H	1:C:2240:HIS:HD2	1.03	0.91
10:B:2406:HOH:O	2:F:2:NAG:O3	1.72	0.90
1:B:1471:GLU:H	1:D:3150:HIS:HE1	1.17	0.88
1:D:3093:LEU:H	1:D:3240:HIS:HD2	1.21	0.88
1:A:150:HIS:HE1	1:C:2471:GLU:H	1.18	0.88
1:C:2093:LEU:H	1:C:2240:HIS:CD2	1.90	0.88
1:B:1207:ASN:HD21	2:E:1:NAG:H2	1.39	0.87
1:B:1406:ASN:ND2	10:B:2330:HOH:O	2.06	0.87
1:A:93:LEU:H	1:A:240:HIS:HD2	1.23	0.87
1:B:1207:ASN:ND2	2:E:1:NAG:H2	1.91	0.86
1:B:1093:LEU:H	1:B:1240:HIS:HD2	1.20	0.85
8:A:1485:MAN:O6	8:A:1486:MAN:C1	2.25	0.84
1:D:3386:VAL:HG22	1:D:3389:ALA:HB2	1.60	0.84
1:C:2150:HIS:HE1	1:D:3471:GLU:H	1.26	0.83
1:C:2281:HIS:HD2	1:C:2301:ASN:H	1.28	0.82
1:D:3233:GLN:HE21	1:D:3247:VAL:H	1.29	0.80
1:B:1233:GLN:HE21	1:B:1247:VAL:H	1.27	0.79
1:C:2233:GLN:HE21	1:C:2247:VAL:H	1.31	0.77
1:B:1281:HIS:HD2	1:B:1301:ASN:H	1.35	0.75
8:A:1485:MAN:O3	8:A:1487:MAN:C1	2.34	0.74
7:B:2483:BMA:C1	2:F:2:NAG:O4	2.36	0.73
1:A:233:GLN:HE21	1:A:247:VAL:H	1.35	0.73
1:D:3281:HIS:HD2	1:D:3301:ASN:H	1.35	0.73
1:B:1207:ASN:HD21	2:E:1:NAG:C2	2.02	0.73
2:H:1:NAG:C4	2:H:2:NAG:C1	2.67	0.71
1:B:1283:GLU:CG	10:B:2218:HOH:O	2.38	0.70
1:C:2207:ASN:ND2	2:H:1:NAG:C1	2.55	0.69
1:A:281:HIS:HD2	1:A:301:ASN:H	1.36	0.69
1:D:3342:ASN:ND2	1:D:3344:ASP:H	1.91	0.69
8:C:3489:MAN:C1	3:G:3:MAN:H3	2.23	0.69
8:C:3489:MAN:C1	3:G:3:MAN:C3	2.71	0.69
1:B:1283:GLU:OE2	10:B:2218:HOH:O	2.11	0.68
2:F:1:NAG:C4	2:F:2:NAG:C1	2.72	0.68
1:C:2332:THR:O	1:C:2333:SER:HB2	1.94	0.68
1:A:93:LEU:H	1:A:240:HIS:CD2	2.11	0.68
1:B:1283:GLU:CD	10:B:2218:HOH:O	2.32	0.67
1:D:3093:LEU:H	1:D:3240:HIS:CD2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3471:GLU:HG3	1:D:3473:ILE:HG22	1.75	0.67
1:A:424:GLU:CD	1:A:424:GLU:H	1.98	0.66
7:B:2483:BMA:O5	2:F:2:NAG:O4	2.13	0.66
1:D:3283:GLU:OE1	10:D:2256:HOH:O	2.11	0.66
1:A:342:ASN:ND2	1:A:344:ASP:H	1.95	0.65
7:C:3490:BMA:C1	2:H:2:NAG:O4	2.44	0.65
1:B:1379:SER:HB2	4:B:2478:SIA:H112	1.79	0.65
1:A:342:ASN:HD22	1:A:344:ASP:H	1.44	0.65
7:A:1484:BMA:C1	2:E:2:NAG:O4	2.45	0.65
1:D:3342:ASN:HD22	1:D:3344:ASP:H	1.45	0.64
1:A:423:LYS:HE3	10:A:2347:HOH:O	1.98	0.64
8:C:3488:MAN:C1	3:G:3:MAN:O6	2.45	0.64
1:C:2233:GLN:NE2	1:C:2247:VAL:H	1.95	0.64
1:B:1405:ASN:C	1:B:1405:ASN:HD22	2.02	0.64
1:D:3424:GLU:H	1:D:3424:GLU:CD	2.00	0.63
1:D:3333:SER:CB	1:D:3353:ASP:O	2.46	0.63
1:B:1093:LEU:H	1:B:1240:HIS:CD2	2.10	0.63
1:D:3333:SER:HB2	1:D:3353:ASP:O	1.98	0.63
7:B:2483:BMA:O6	8:B:2484:MAN:C1	2.46	0.63
1:C:2093:LEU:N	1:C:2240:HIS:HD2	1.87	0.63
1:A:150:HIS:CE1	1:C:2471:GLU:H	2.09	0.62
1:A:460:ARG:HD2	10:A:2420:HOH:O	1.98	0.62
1:B:1207:ASN:HD21	2:E:1:NAG:C1	2.14	0.61
1:C:2204:PRO:HD3	1:D:3464:TRP:HB3	1.81	0.61
1:D:3283:GLU:CD	10:D:2256:HOH:O	2.39	0.61
1:A:124:ARG:HA	1:A:449:ASN:ND2	2.15	0.61
1:B:1375:LYS:NZ	10:B:2302:HOH:O	2.32	0.61
1:A:473:ILE:HG12	10:A:2389:HOH:O	2.00	0.61
1:D:3207:ASN:OD1	2:F:1:NAG:C1	2.49	0.61
5:A:1479:GOL:H32	1:C:2113:ARG:NH2	2.16	0.61
1:D:3332:THR:O	1:D:3333:SER:HB2	2.00	0.61
1:C:2424:GLU:CD	1:C:2424:GLU:H	2.03	0.60
8:C:3489:MAN:C1	3:G:3:MAN:O3	2.49	0.60
1:B:1342:ASN:HD22	1:B:1344:ASP:H	1.48	0.60
1:A:293:VAL:HG22	10:A:2224:HOH:O	2.02	0.60
4:A:1478:SIA:H6	4:A:1478:SIA:O1A	2.00	0.59
1:B:1127:TYR:CG	1:B:1235:SER:HA	2.37	0.59
1:B:1342:ASN:ND2	1:B:1344:ASP:H	2.01	0.59
1:A:467:HIS:CD2	1:A:467:HIS:H	2.20	0.58
1:C:2150:HIS:CE1	1:D:3471:GLU:H	2.15	0.58
1:C:2465:SER:OG	1:C:2467:HIS:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3283:GLU:CG	10:D:2256:HOH:O	2.51	0.58
1:A:445:LEU:HD21	6:A:1481:NAG:H82	1.86	0.58
1:B:1333:SER:CB	1:B:1353:ASP:O	2.51	0.58
1:B:1131:ASP:HB2	1:B:1132:PRO:CD	2.34	0.58
7:A:1484:BMA:O6	8:A:1485:MAN:C1	2.52	0.57
1:D:3281:HIS:CD2	1:D:3301:ASN:H	2.17	0.57
1:B:1379:SER:HB2	4:B:2478:SIA:C11	2.36	0.56
1:B:1379:SER:OG	1:B:1406:ASN:ND2	2.38	0.56
1:B:1465:SER:OG	1:B:1467:HIS:HD2	1.88	0.56
7:A:1484:BMA:O5	2:E:2:NAG:O4	2.22	0.56
1:C:2409:TRP:CZ3	4:C:3478:SIA:H112	2.41	0.56
7:C:3490:BMA:C1	2:H:2:NAG:HO4	2.18	0.56
1:C:2281:HIS:CD2	1:C:2301:ASN:H	2.17	0.55
5:C:3479:GOL:H32	1:D:3113:ARG:NH2	2.21	0.55
8:C:3485:MAN:C1	3:G:2:BMA:O3	2.54	0.55
1:B:1113:ARG:NH2	5:D:4479:GOL:H32	2.21	0.55
1:B:1156:HIS:HB2	10:B:2083:HOH:O	2.06	0.55
1:B:1461:LEU:O	2:F:1:NAG:H62	2.07	0.55
1:D:3207:ASN:CG	2:F:1:NAG:C1	2.76	0.55
1:B:1283:GLU:HG3	10:B:2218:HOH:O	2.05	0.54
1:B:1460:ARG:NH1	10:B:2368:HOH:O	2.37	0.54
1:A:332:THR:O	1:A:333:SER:HB2	2.08	0.54
1:C:2409:TRP:CE3	4:C:3478:SIA:H112	2.43	0.54
1:C:2150:HIS:HE1	1:D:3471:GLU:N	2.03	0.54
1:D:3088:ARG:NH2	1:D:3133:GLN:OE1	2.39	0.54
4:A:1477:SIA:O2	4:A:1477:SIA:H5	2.09	0.53
4:B:2477:SIA:H5	4:B:2477:SIA:O2	2.09	0.53
7:C:3490:BMA:C1	2:H:2:NAG:C4	2.87	0.53
1:D:3369:LEU:HG	1:D:3386:VAL:HG13	1.89	0.53
1:B:1207:ASN:ND2	2:E:1:NAG:C2	2.67	0.53
1:B:1256:ARG:HD3	10:B:2191:HOH:O	2.08	0.53
1:D:3207:ASN:HD21	2:F:1:NAG:C7	2.21	0.53
4:D:4477:SIA:H5	4:D:4477:SIA:O2	2.09	0.53
1:A:156:HIS:HB2	10:A:2068:HOH:O	2.07	0.53
4:C:3477:SIA:H5	4:C:3477:SIA:O2	2.09	0.53
1:B:1471:GLU:H	1:D:3150:HIS:CE1	2.10	0.52
1:D:3342:ASN:HD22	1:D:3342:ASN:C	2.12	0.52
1:A:92:ASN:CG	6:A:1480:NAG:C1	2.74	0.52
1:A:424:GLU:CD	1:A:424:GLU:N	2.63	0.52
1:C:2297:ILE:N	1:C:2297:ILE:HD12	2.25	0.52
7:A:1484:BMA:C1	2:E:2:NAG:C4	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASN:HD22	1:A:342:ASN:C	2.14	0.51
1:C:2235:SER:HB3	1:C:2357:LYS:HE2	1.92	0.51
1:B:1333:SER:HB3	1:B:1353:ASP:O	2.10	0.51
1:B:1423:LYS:HE2	10:D:2190:HOH:O	2.10	0.51
1:D:3204:PRO:HG2	1:D:3207:ASN:HB2	1.93	0.51
1:D:3233:GLN:NE2	1:D:3247:VAL:H	2.02	0.51
1:B:1332:THR:O	1:B:1333:SER:HB2	2.10	0.51
4:D:4478:SIA:O1A	4:D:4478:SIA:H6	2.09	0.51
1:A:333:SER:CB	1:A:353:ASP:O	2.59	0.50
8:C:3485:MAN:C1	3:G:2:BMA:C3	2.89	0.50
1:B:1195:SER:HB2	1:B:1214:TYR:CZ	2.47	0.50
1:A:235:SER:HB3	1:A:357:LYS:HE2	1.93	0.50
7:A:1484:BMA:C1	2:E:2:NAG:H4	2.42	0.50
1:A:333:SER:HB2	1:A:353:ASP:O	2.11	0.49
1:C:2124:ARG:HA	1:C:2449:ASN:ND2	2.27	0.49
1:D:3231:ARG:NE	1:D:3283:GLU:OE2	2.42	0.49
8:A:1485:MAN:O3	8:A:1487:MAN:H5	2.11	0.49
8:C:3486:MAN:H62	10:C:3418:HOH:O	2.11	0.49
1:D:3471:GLU:OE2	1:D:3473:ILE:HG22	2.12	0.49
1:A:465:SER:OG	1:A:467:HIS:HD2	1.94	0.49
1:B:1333:SER:HB2	1:B:1353:ASP:O	2.12	0.49
1:D:3471:GLU:CG	1:D:3473:ILE:HG22	2.42	0.49
1:C:2333:SER:CB	1:C:2353:ASP:O	2.61	0.49
1:C:2240:HIS:HE1	1:C:2315:GLU:OE1	1.95	0.49
4:D:4477:SIA:O2	4:D:4477:SIA:C5	2.59	0.49
4:A:1477:SIA:O2	4:A:1477:SIA:C5	2.59	0.48
1:C:2375:LYS:HG2	10:C:3307:HOH:O	2.13	0.48
1:D:3333:SER:HB3	1:D:3353:ASP:O	2.13	0.48
3:G:1:NAG:C4	3:G:2:BMA:C1	2.91	0.48
1:D:3235:SER:HB3	1:D:3357:LYS:HE2	1.95	0.48
1:A:324:LEU:HD21	1:A:362:LEU:HD21	1.96	0.48
1:A:93:LEU:N	1:A:240:HIS:HD2	2.03	0.48
1:A:240:HIS:HE1	1:A:315:GLU:OE2	1.96	0.48
1:A:417:ILE:HG21	1:A:426:PHE:HB3	1.95	0.48
1:C:2127:TYR:CG	1:C:2235:SER:HA	2.49	0.47
1:B:1156:HIS:CE1	10:B:2082:HOH:O	2.66	0.47
1:D:3097:LEU:HD22	1:D:3428:PRO:HG3	1.96	0.47
1:A:460:ARG:O	1:A:460:ARG:HG3	2.14	0.47
1:B:1285:CYS:HB3	1:B:1296:CYS:HB3	1.97	0.47
1:D:3283:GLU:HG3	10:D:2256:HOH:O	2.14	0.47
1:B:1445:LEU:HD11	6:B:2480:NAG:H82	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2473:ILE:HG12	10:C:3387:HOH:O	2.13	0.47
1:D:3131:ASP:HB2	1:D:3132:PRO:CD	2.44	0.47
1:D:3341:GLY:HA2	1:D:3347:ILE:HD11	1.96	0.47
4:B:2478:SIA:O1A	4:B:2478:SIA:H6	2.15	0.47
1:B:1281:HIS:CD2	1:B:1301:ASN:H	2.23	0.46
1:B:1342:ASN:HD22	1:B:1342:ASN:C	2.18	0.46
1:B:1374:SER:N	10:B:2330:HOH:O	2.44	0.46
1:A:417:ILE:HB	1:A:419:TYR:CZ	2.51	0.46
1:C:2333:SER:HB2	1:C:2353:ASP:O	2.15	0.46
1:D:3445:LEU:HD21	6:D:4480:NAG:H82	1.98	0.46
2:F:1:NAG:O4	2:F:2:NAG:H83	2.15	0.46
1:D:3240:HIS:HE1	1:D:3315:GLU:OE1	1.99	0.45
1:D:3461:LEU:O	2:H:1:NAG:H62	2.15	0.45
1:D:3131:ASP:HB2	1:D:3132:PRO:HD2	1.96	0.45
1:C:2207:ASN:CG	2:H:1:NAG:C1	2.84	0.45
1:C:2417:ILE:HB	1:C:2419:TYR:CZ	2.52	0.45
1:A:330:THR:HG21	1:A:369:LEU:HB3	1.99	0.45
8:C:3485:MAN:C1	3:G:2:BMA:H3	2.47	0.45
7:A:1484:BMA:C1	2:E:2:NAG:HO4	2.25	0.44
1:C:2115:GLY:HA2	1:C:2120:ILE:HG12	1.99	0.44
1:D:3117:ASP:CG	1:D:3117:ASP:O	2.55	0.44
1:B:1235:SER:HB3	1:B:1357:LYS:HE2	1.98	0.44
1:C:2102:SER:HB2	1:C:2459:LYS:O	2.18	0.44
1:A:400:ASN:HB3	8:A:1485:MAN:C1	2.48	0.44
1:B:1417:ILE:HG21	1:B:1426:PHE:HB3	1.99	0.44
1:C:2427:ASN:HA	1:C:2428:PRO:HD3	1.88	0.44
4:D:4477:SIA:O2	4:D:4477:SIA:O7	2.30	0.44
1:A:97:LEU:HD12	1:A:363:ASP:HB2	1.99	0.44
1:C:2150:HIS:CE1	1:D:3470:ALA:HA	2.52	0.43
1:A:229:ILE:HG22	1:A:229:ILE:O	2.18	0.43
1:C:2285:CYS:HB3	1:C:2296:CYS:HB3	1.99	0.43
2:F:1:NAG:H4	2:F:2:NAG:C1	2.48	0.43
1:D:3297:ILE:N	1:D:3297:ILE:HD12	2.32	0.43
1:B:1124:ARG:HA	1:B:1449:ASN:ND2	2.34	0.43
1:D:3124:ARG:HA	1:D:3449:ASN:ND2	2.33	0.43
1:B:1240:HIS:HE1	1:B:1315:GLU:OE2	2.02	0.43
1:C:2150:HIS:HD2	10:D:2088:HOH:O	2.01	0.43
1:C:2156:HIS:CE1	10:C:3097:HOH:O	2.71	0.43
1:C:2357:LYS:HB3	1:C:2412:TYR:CG	2.54	0.43
1:C:2445:LEU:HD21	6:C:3481:NAG:H82	2.01	0.43
1:B:1467:HIS:CD2	1:B:1467:HIS:H	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1:NAG:HO4	3:G:2:BMA:C1	2.24	0.42
1:A:150:HIS:HE1	1:C:2471:GLU:N	2.00	0.42
1:A:233:GLN:NE2	1:A:247:VAL:H	2.11	0.42
1:D:3342:ASN:HD22	1:D:3343:CYS:N	2.18	0.42
1:C:2131:ASP:HB2	1:C:2132:PRO:CD	2.50	0.42
4:C:3477:SIA:O2	4:C:3477:SIA:C5	2.59	0.42
1:A:235:SER:HB3	1:A:357:LYS:CE	2.50	0.42
8:A:1485:MAN:C3	8:A:1487:MAN:C1	2.97	0.42
8:C:3485:MAN:O2	8:C:3486:MAN:C1	2.68	0.42
10:C:3413:HOH:O	2:H:2:NAG:O3	2.21	0.42
1:D:3386:VAL:HG23	1:D:3395:SER:HB2	2.01	0.42
1:C:2325:CYS:O	1:C:2393:ILE:HA	2.19	0.41
1:C:2351:SER:HA	1:C:2352:PRO:HA	1.78	0.41
5:A:1479:GOL:H32	1:C:2113:ARG:HH22	1.82	0.41
1:A:204:PRO:HD3	1:C:2464:TRP:HB3	2.03	0.41
1:B:1464:TRP:HB3	1:D:3204:PRO:HD3	2.03	0.41
1:D:3156:HIS:CE1	10:D:2134:HOH:O	2.74	0.41
1:A:165:ILE:HA	1:A:179:ARG:O	2.20	0.41
1:B:1233:GLN:NE2	1:B:1247:VAL:H	2.05	0.41
1:C:2197:MET:HA	1:C:2213:TRP:O	2.21	0.41
1:A:150:HIS:HD2	10:C:3047:HOH:O	2.04	0.41
1:A:197:MET:HA	1:A:213:TRP:O	2.21	0.41
1:A:332:THR:HB	1:A:356:VAL:CG1	2.50	0.41
4:A:1477:SIA:O2	4:A:1477:SIA:O7	2.30	0.41
7:C:3490:BMA:C1	2:H:2:NAG:H4	2.51	0.41
1:A:88:ARG:HH12	1:A:133:GLN:HE22	1.69	0.41
1:A:282:ILE:HD12	1:A:310:ILE:HD11	2.02	0.41
1:C:2218:PRO:HB2	10:C:3166:HOH:O	2.21	0.41
1:D:3195:SER:HB2	1:D:3214:TYR:CZ	2.56	0.41
1:A:124:ARG:HA	1:A:449:ASN:HD22	1.85	0.40
1:B:1307:ARG:HA	1:B:1308:PRO:HD3	1.94	0.40
1:A:113:ARG:NH2	5:B:2479:GOL:H32	2.36	0.40
1:C:2340:ASN:ND2	10:C:3269:HOH:O	2.53	0.40
8:C:3485:MAN:H5	3:G:2:BMA:H2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/389 (100%)	368 (95%)	18 (5%)	1 (0%)	41	39
1	B	387/389 (100%)	372 (96%)	14 (4%)	1 (0%)	41	39
1	C	387/389 (100%)	367 (95%)	19 (5%)	1 (0%)	41	39
1	D	387/389 (100%)	372 (96%)	15 (4%)	0	100	100
All	All	1548/1556 (100%)	1479 (96%)	66 (4%)	3 (0%)	47	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	SER
1	B	1333	SER
1	C	2333	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	331/331 (100%)	326 (98%)	5 (2%)	65	69
1	B	331/331 (100%)	321 (97%)	10 (3%)	41	43
1	C	331/331 (100%)	326 (98%)	5 (2%)	65	69
1	D	331/331 (100%)	324 (98%)	7 (2%)	53	57
All	All	1324/1324 (100%)	1297 (98%)	27 (2%)	55	59

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	342	ASN
1	A	445	LEU
1	A	460	ARG
1	A	464	TRP
1	B	1088	ARG
1	B	1128	LEU
1	B	1142	GLN
1	B	1185	TRP
1	B	1256	ARG
1	B	1333	SER
1	B	1342	ASN
1	B	1405	ASN
1	B	1422	ASN
1	B	1464	TRP
1	C	2128	LEU
1	C	2333	SER
1	C	2424	GLU
1	C	2445	LEU
1	C	2464	TRP
1	D	3128	LEU
1	D	3237	CYS
1	D	3342	ASN
1	D	3386	VAL
1	D	3424	GLU
1	D	3445	LEU
1	D	3464	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	150	HIS
1	A	152	ASN
1	A	233	GLN
1	A	240	HIS
1	A	281	HIS
1	A	340	ASN
1	A	342	ASN
1	A	406	ASN
1	A	408	ASN
1	A	422	ASN
1	A	427	ASN

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Mol	Chain	Res	Type
1	A	449	ASN
1	A	467	HIS
1	B	1142	GLN
1	B	1152	ASN
1	B	1207	ASN
1	B	1233	GLN
1	B	1240	HIS
1	B	1281	HIS
1	B	1340	ASN
1	B	1342	ASN
1	B	1400	ASN
1	B	1405	ASN
1	B	1406	ASN
1	B	1408	ASN
1	B	1422	ASN
1	B	1427	ASN
1	B	1449	ASN
1	B	1467	HIS
1	C	2150	HIS
1	C	2152	ASN
1	C	2207	ASN
1	C	2233	GLN
1	C	2240	HIS
1	C	2270	GLN
1	C	2281	HIS
1	C	2340	ASN
1	C	2406	ASN
1	C	2408	ASN
1	C	2422	ASN
1	C	2427	ASN
1	C	2449	ASN
1	C	2467	HIS
1	D	3150	HIS
1	D	3152	ASN
1	D	3207	ASN
1	D	3233	GLN
1	D	3240	HIS
1	D	3281	HIS
1	D	3340	ASN
1	D	3342	ASN
1	D	3406	ASN
1	D	3422	ASN

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Mol	Chain	Res	Type
1	D	3427	ASN
1	D	3449	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

9 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	E	1	2	14,14,15	0.27	0	17,19,21	1.02	1 (5%)
2	NAG	E	2	2	14,14,15	0.27	0	17,19,21	1.01	1 (5%)
2	NAG	F	1	2	14,14,15	0.26	0	17,19,21	1.00	1 (5%)
2	NAG	F	2	2	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
3	NAG	G	1	3	14,14,15	0.27	0	17,19,21	1.02	1 (5%)
3	BMA	G	2	3	11,11,12	0.27	0	15,15,17	0.64	0
3	MAN	G	3	3	11,11,12	0.26	0	15,15,17	0.64	0
2	NAG	H	1	2	14,14,15	0.27	0	17,19,21	1.02	1 (5%)
2	NAG	H	2	2	14,14,15	0.27	0	17,19,21	1.01	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	1	2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	1/6/23/26	0/1/1/1
2	NAG	F	1	2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
3	NAG	G	1	3	-	2/6/23/26	0/1/1/1
3	BMA	G	2	3	-	2/2/19/22	0/1/1/1
3	MAN	G	3	3	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	C1-C2-N2	-3.22	104.98	110.49
2	H	1	NAG	C1-C2-N2	-3.22	104.99	110.49
2	H	2	NAG	C1-C2-N2	-3.21	105.01	110.49
2	E	2	NAG	C1-C2-N2	-3.21	105.01	110.49
2	E	1	NAG	C1-C2-N2	-3.20	105.03	110.49
2	F	2	NAG	C1-C2-N2	-3.19	105.05	110.49
2	F	1	NAG	C1-C2-N2	-3.17	105.08	110.49

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
3	G	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	G	2	BMA	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	G	2	BMA	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	2	NAG	7	0
3	G	3	MAN	4	0
3	G	1	NAG	2	0
2	E	2	NAG	5	0
2	E	1	NAG	5	0
2	H	1	NAG	5	0
3	G	2	BMA	6	0
2	F	1	NAG	7	0
2	F	2	NAG	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain H

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain G

Bond lengths

Bond angles

Torsions

Rings
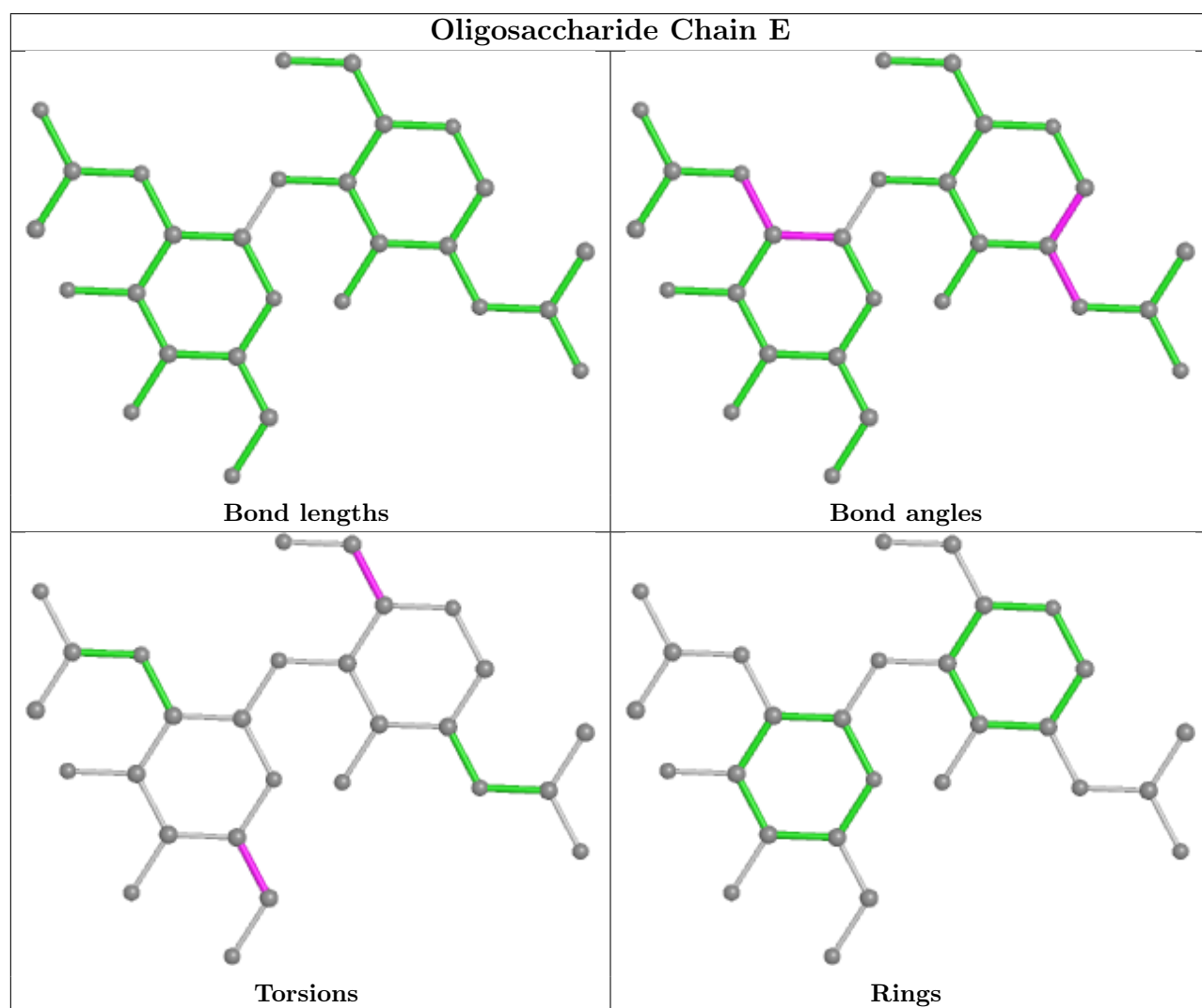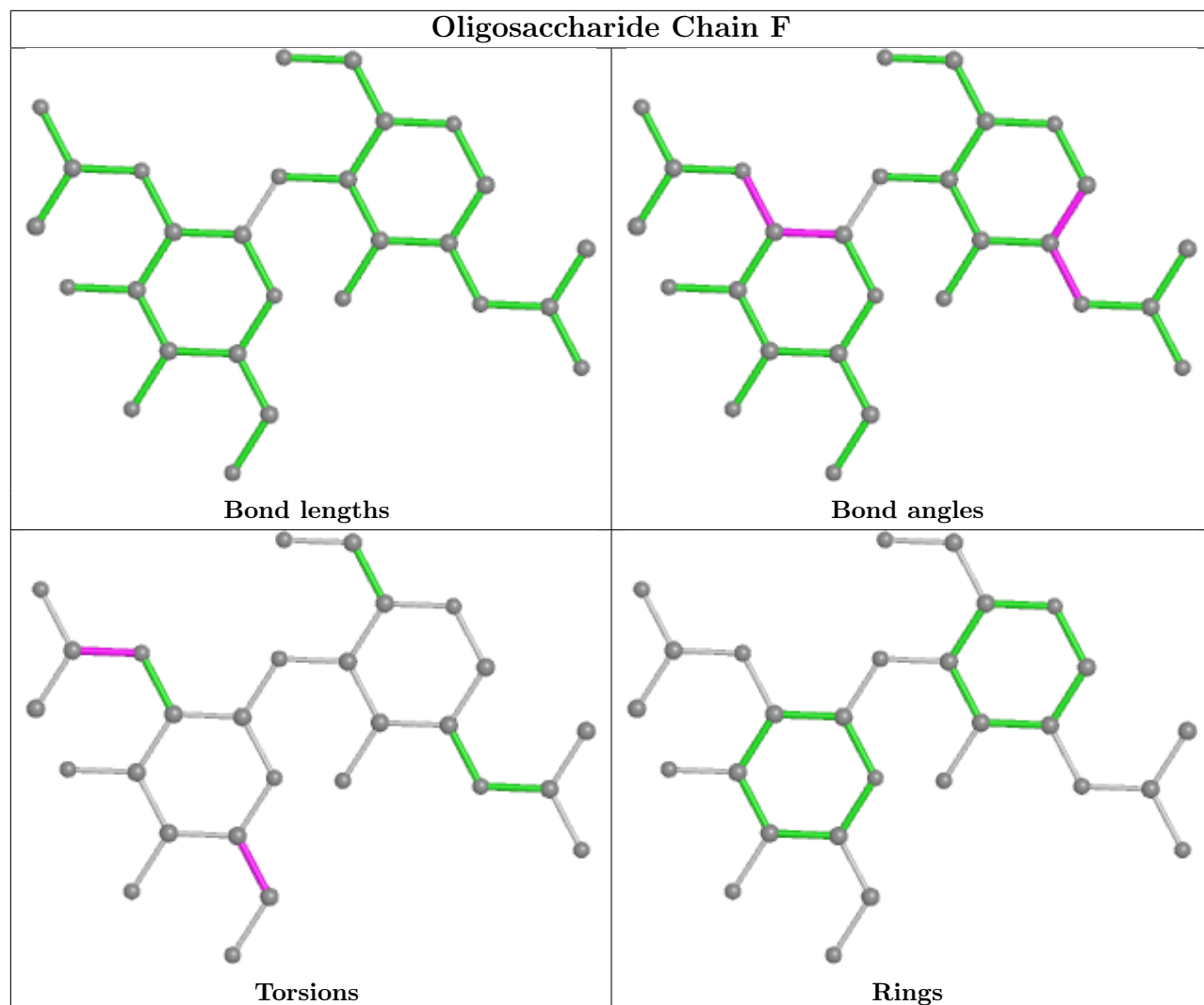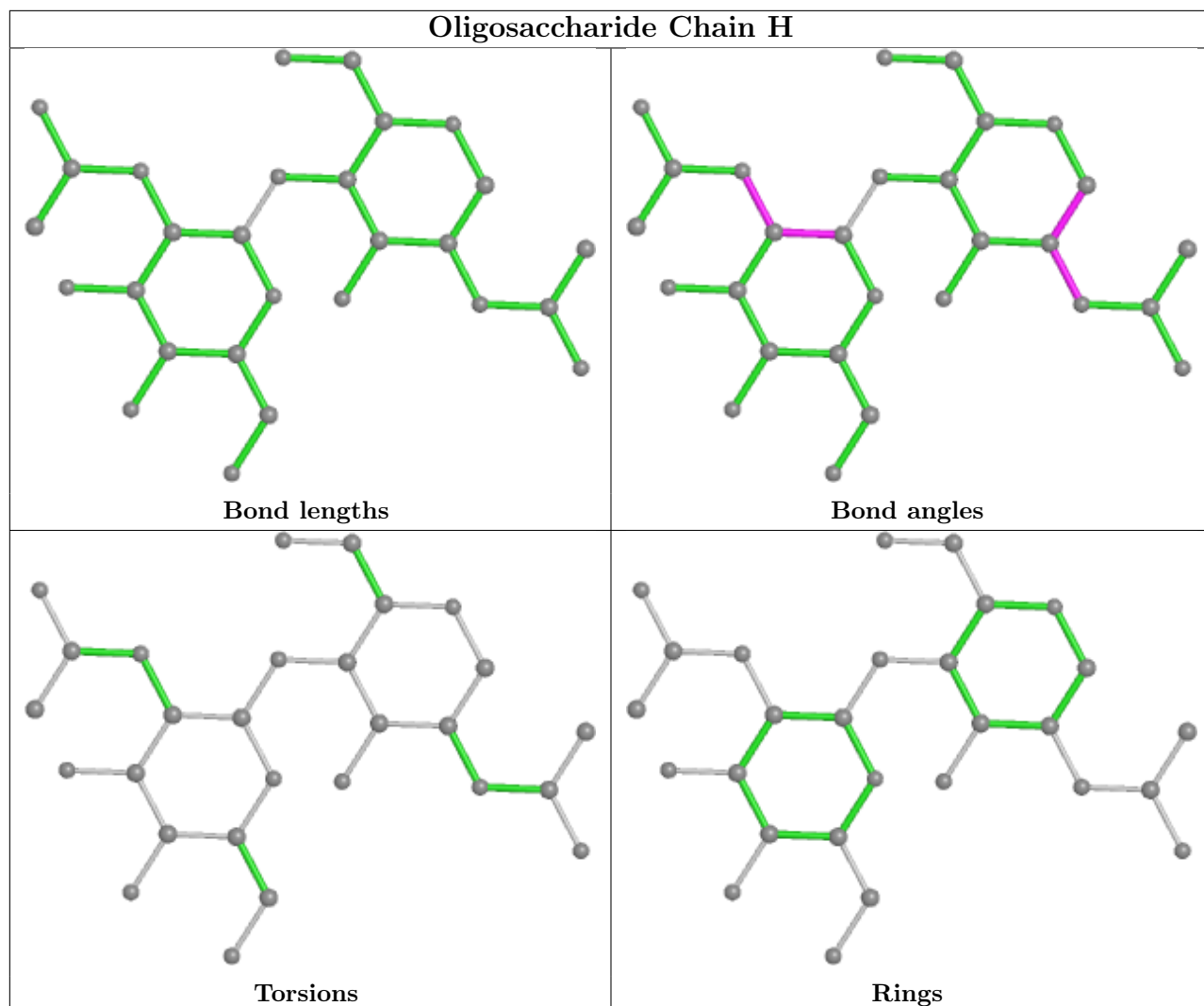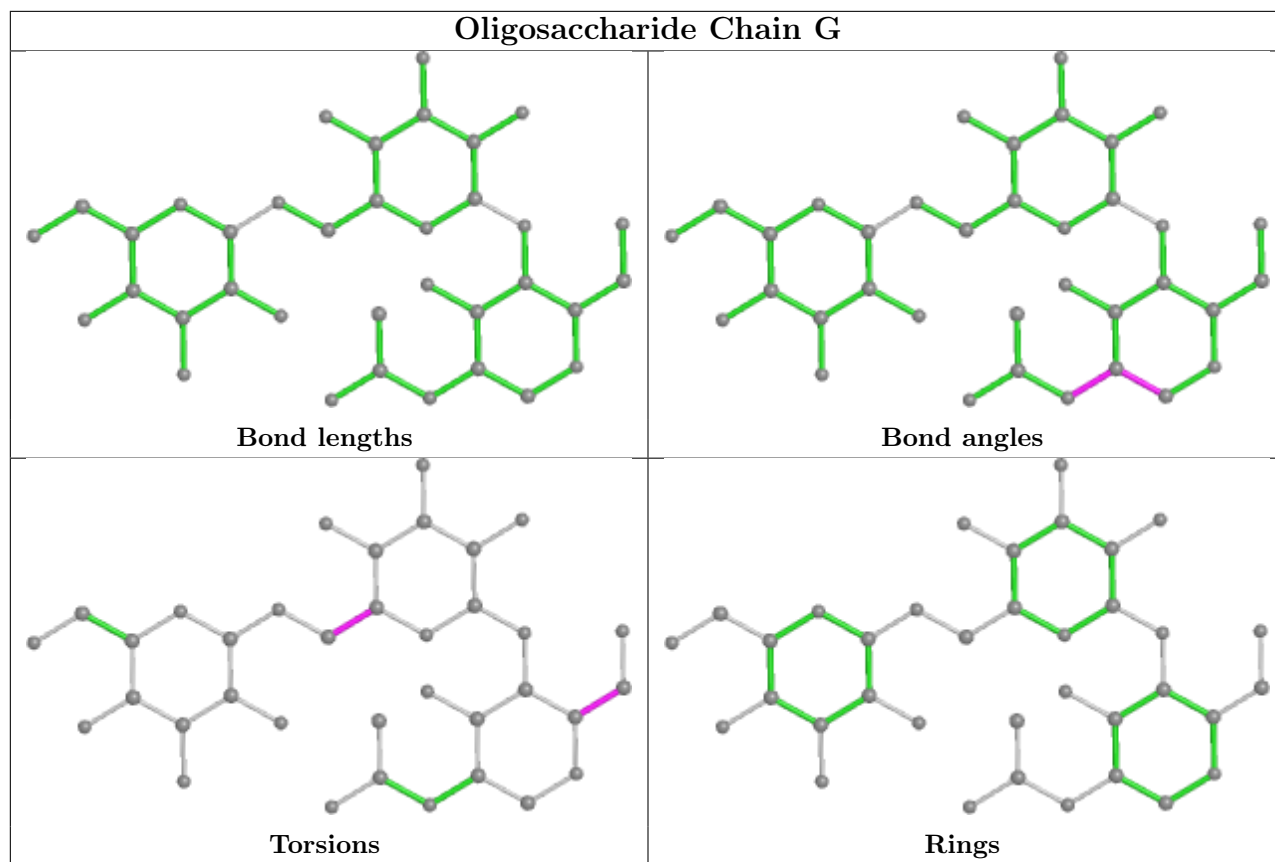
5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	SIA	D	4477	-	21,21,21	0.89	1 (4%)	25,31,31	1.30	3 (12%)
8	MAN	C	3485	-	11,11,12	0.26	0	15,15,17	0.63	0
6	NAG	C	3481	-	14,14,15	0.28	0	17,19,21	1.01	1 (5%)
5	GOL	B	2479	-	5,5,5	3.18	2 (40%)	5,5,5	6.21	4 (80%)
8	MAN	C	3488	-	11,11,12	0.26	0	15,15,17	0.64	0
8	MAN	C	3489	-	11,11,12	0.26	0	15,15,17	0.64	0
7	BMA	A	1484	-	11,11,12	0.26	0	15,15,17	0.63	0
8	MAN	A	1487	-	11,11,12	0.26	0	15,15,17	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
8	MAN	C	3486	-	11,11,12	0.26	0	15,15,17	0.64	0
6	NAG	B	2480	-	14,14,15	0.26	0	17,19,21	1.01	1 (5%)
7	BMA	B	2483	-	11,11,12	0.26	0	15,15,17	0.64	0
8	MAN	B	2484	-	11,11,12	0.27	0	15,15,17	0.63	0
6	NAG	D	4480	-	14,14,15	0.25	0	17,19,21	1.01	1 (5%)
4	SIA	C	3477	-	21,21,21	0.90	1 (4%)	25,31,31	1.30	3 (12%)
8	MAN	B	2486	-	11,11,12	0.28	0	15,15,17	0.64	0
8	MAN	A	1485	-	11,11,12	0.26	0	15,15,17	0.64	0
5	GOL	D	4479	-	5,5,5	3.50	2 (40%)	5,5,5	6.50	4 (80%)
4	SIA	B	2478	-	21,21,21	0.92	1 (4%)	25,31,31	1.29	3 (12%)
4	SIA	A	1477	-	21,21,21	0.89	1 (4%)	25,31,31	1.30	3 (12%)
5	GOL	A	1479	-	5,5,5	3.60	2 (40%)	5,5,5	6.34	4 (80%)
8	MAN	B	2485	-	11,11,12	0.26	0	15,15,17	0.63	0
4	SIA	D	4478	-	21,21,21	0.90	1 (4%)	25,31,31	1.29	3 (12%)
4	SIA	C	3478	-	21,21,21	0.89	1 (4%)	25,31,31	1.29	3 (12%)
5	GOL	C	3479	-	5,5,5	3.33	3 (60%)	5,5,5	6.32	4 (80%)
8	MAN	A	1486	-	11,11,12	0.27	0	15,15,17	0.64	0
4	SIA	A	1478	-	21,21,21	0.91	1 (4%)	25,31,31	1.29	3 (12%)
4	SIA	B	2477	-	21,21,21	0.89	1 (4%)	25,31,31	1.31	3 (12%)
6	NAG	A	1480	1	14,14,15	0.26	0	17,19,21	1.02	1 (5%)
6	NAG	A	1481	-	14,14,15	0.27	0	17,19,21	1.00	1 (5%)
7	BMA	C	3490	-	11,11,12	0.26	0	15,15,17	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SIA	D	4477	-	-	2/20/38/38	0/1/1/1
8	MAN	C	3485	-	-	1/2/19/22	0/1/1/1
6	NAG	C	3481	-	-	2/6/23/26	0/1/1/1
5	GOL	B	2479	-	-	2/4/4/4	-
8	MAN	C	3488	-	-	2/2/19/22	0/1/1/1
8	MAN	C	3489	-	-	0/2/19/22	0/1/1/1
7	BMA	A	1484	-	-	2/2/19/22	0/1/1/1
8	MAN	A	1487	-	-	1/2/19/22	0/1/1/1
8	MAN	C	3486	-	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	2480	-	-	2/6/23/26	0/1/1/1
7	BMA	B	2483	-	-	0/2/19/22	0/1/1/1
8	MAN	B	2484	-	-	0/2/19/22	0/1/1/1
6	NAG	D	4480	-	-	0/6/23/26	0/1/1/1
4	SIA	C	3477	-	-	2/20/38/38	0/1/1/1
8	MAN	B	2486	-	-	0/2/19/22	0/1/1/1
8	MAN	A	1485	-	-	0/2/19/22	0/1/1/1
5	GOL	D	4479	-	-	2/4/4/4	-
4	SIA	B	2478	-	-	0/20/38/38	0/1/1/1
4	SIA	A	1477	-	-	2/20/38/38	0/1/1/1
5	GOL	A	1479	-	-	2/4/4/4	-
8	MAN	B	2485	-	-	2/2/19/22	0/1/1/1
4	SIA	D	4478	-	-	0/20/38/38	0/1/1/1
4	SIA	C	3478	-	-	4/20/38/38	0/1/1/1
5	GOL	C	3479	-	-	3/4/4/4	-
8	MAN	A	1486	-	-	2/2/19/22	0/1/1/1
4	SIA	A	1478	-	-	0/20/38/38	0/1/1/1
4	SIA	B	2477	-	-	3/20/38/38	0/1/1/1
6	NAG	A	1480	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1481	-	-	1/6/23/26	0/1/1/1
7	BMA	C	3490	-	-	0/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1479	GOL	O1-C1	-5.53	1.19	1.42
5	A	1479	GOL	C1-C2	-5.45	1.29	1.51
5	D	4479	GOL	O1-C1	-5.36	1.19	1.42
5	D	4479	GOL	C1-C2	-5.21	1.30	1.51
5	C	3479	GOL	C1-C2	-5.03	1.31	1.51
5	C	3479	GOL	O1-C1	-4.87	1.21	1.42
5	B	2479	GOL	O1-C1	-4.86	1.21	1.42
5	B	2479	GOL	C1-C2	-4.73	1.32	1.51
4	B	2478	SIA	O2-C2	3.21	1.43	1.39
4	C	3477	SIA	O2-C2	3.16	1.43	1.39
4	A	1478	SIA	O2-C2	3.16	1.43	1.39
4	D	4477	SIA	O2-C2	3.13	1.43	1.39
4	C	3478	SIA	O2-C2	3.13	1.43	1.39
4	D	4478	SIA	O2-C2	3.10	1.43	1.39
4	A	1477	SIA	O2-C2	3.10	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2477	SIA	O2-C2	3.09	1.43	1.39
5	C	3479	GOL	C3-C2	-2.43	1.41	1.51

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	4479	GOL	O1-C1-C2	12.10	168.22	110.20
5	A	1479	GOL	O1-C1-C2	11.88	167.15	110.20
5	C	3479	GOL	O1-C1-C2	11.85	167.04	110.20
5	B	2479	GOL	O1-C1-C2	11.37	164.73	110.20
5	B	2479	GOL	O3-C3-C2	6.31	140.44	110.20
5	D	4479	GOL	O3-C3-C2	6.29	140.36	110.20
5	A	1479	GOL	O3-C3-C2	5.84	138.21	110.20
5	C	3479	GOL	O3-C3-C2	5.55	136.83	110.20
5	A	1479	GOL	O2-C2-C3	4.02	126.81	109.12
5	C	3479	GOL	O2-C2-C1	4.01	126.79	109.12
5	B	2479	GOL	O2-C2-C1	3.69	125.38	109.12
4	C	3477	SIA	C6-C5-N5	-3.58	104.97	110.91
4	B	2477	SIA	C6-C5-N5	-3.57	104.98	110.91
4	A	1477	SIA	C6-C5-N5	-3.57	104.98	110.91
4	C	3478	SIA	C6-C5-N5	-3.57	104.99	110.91
4	D	4478	SIA	C6-C5-N5	-3.57	104.99	110.91
4	B	2478	SIA	C6-C5-N5	-3.56	105.00	110.91
4	D	4477	SIA	C6-C5-N5	-3.56	105.00	110.91
5	D	4479	GOL	O2-C2-C3	3.55	124.75	109.12
4	A	1478	SIA	C6-C5-N5	-3.54	105.03	110.91
5	D	4479	GOL	O2-C2-C1	3.53	124.69	109.12
4	B	2477	SIA	O1A-C1-C2	-3.40	118.44	123.59
5	C	3479	GOL	O2-C2-C3	3.39	124.06	109.12
4	D	4477	SIA	O1A-C1-C2	-3.38	118.47	123.59
4	A	1478	SIA	O1A-C1-C2	-3.36	118.49	123.59
4	B	2478	SIA	O1A-C1-C2	-3.36	118.50	123.59
4	C	3478	SIA	O1A-C1-C2	-3.35	118.51	123.59
4	A	1477	SIA	O1A-C1-C2	-3.35	118.52	123.59
4	C	3477	SIA	O1A-C1-C2	-3.35	118.52	123.59
4	D	4478	SIA	O1A-C1-C2	-3.33	118.54	123.59
5	B	2479	GOL	O2-C2-C3	3.22	123.32	109.12
6	A	1480	NAG	C1-C2-N2	-3.22	104.98	110.49
6	A	1481	NAG	C1-C2-N2	-3.21	105.01	110.49
6	D	4480	NAG	C1-C2-N2	-3.20	105.03	110.49
6	B	2480	NAG	C1-C2-N2	-3.19	105.03	110.49
6	C	3481	NAG	C1-C2-N2	-3.19	105.03	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1479	GOL	O2-C2-C1	3.11	122.82	109.12
4	B	2478	SIA	C4-C5-N5	-2.73	104.98	110.38
4	C	3478	SIA	C4-C5-N5	-2.73	104.98	110.38
4	C	3477	SIA	C4-C5-N5	-2.72	104.99	110.38
4	B	2477	SIA	C4-C5-N5	-2.71	105.01	110.38
4	A	1478	SIA	C4-C5-N5	-2.71	105.01	110.38
4	D	4478	SIA	C4-C5-N5	-2.71	105.01	110.38
4	D	4477	SIA	C4-C5-N5	-2.70	105.03	110.38
4	A	1477	SIA	C4-C5-N5	-2.70	105.04	110.38

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3477	SIA	O1B-C1-C2-O6
4	C	3478	SIA	O1B-C1-C2-O6
5	A	1479	GOL	O1-C1-C2-C3
5	A	1479	GOL	O2-C2-C3-O3
5	B	2479	GOL	O1-C1-C2-C3
5	C	3479	GOL	O1-C1-C2-O2
5	D	4479	GOL	O1-C1-C2-C3
8	B	2485	MAN	O5-C5-C6-O6
8	A	1486	MAN	C4-C5-C6-O6
8	A	1486	MAN	O5-C5-C6-O6
8	B	2485	MAN	C4-C5-C6-O6
6	B	2480	NAG	O5-C5-C6-O6
8	C	3488	MAN	O5-C5-C6-O6
6	B	2480	NAG	C4-C5-C6-O6
8	C	3488	MAN	C4-C5-C6-O6
7	A	1484	BMA	O5-C5-C6-O6
5	C	3479	GOL	O2-C2-C3-O3
7	A	1484	BMA	C4-C5-C6-O6
5	C	3479	GOL	O1-C1-C2-C3
5	B	2479	GOL	O2-C2-C3-O3
5	D	4479	GOL	O2-C2-C3-O3
6	C	3481	NAG	C4-C5-C6-O6
6	C	3481	NAG	O5-C5-C6-O6
4	B	2477	SIA	O1A-C1-C2-O6
4	C	3478	SIA	O1A-C1-C2-O6
8	A	1487	MAN	C4-C5-C6-O6
4	B	2477	SIA	O1A-C1-C2-C3
4	C	3478	SIA	O1A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	3477	SIA	O1A-C1-C2-O6
6	A	1481	NAG	C4-C5-C6-O6
4	A	1477	SIA	O1A-C1-C2-O2
4	B	2477	SIA	O1A-C1-C2-O2
4	C	3478	SIA	O1A-C1-C2-O2
4	D	4477	SIA	O1A-C1-C2-O2
4	A	1477	SIA	O1B-C1-C2-O6
4	D	4477	SIA	O1B-C1-C2-O6
8	C	3485	MAN	O5-C5-C6-O6

There are no ring outliers.

29 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4477	SIA	3	0
8	C	3485	MAN	5	0
6	C	3481	NAG	3	0
5	B	2479	GOL	1	0
8	C	3488	MAN	1	0
8	C	3489	MAN	3	0
7	A	1484	BMA	6	0
8	A	1487	MAN	3	0
8	C	3486	MAN	2	0
6	B	2480	NAG	3	0
7	B	2483	BMA	3	0
8	B	2484	MAN	2	0
6	D	4480	NAG	3	0
4	C	3477	SIA	2	0
8	A	1485	MAN	6	0
5	D	4479	GOL	1	0
4	B	2478	SIA	3	0
4	A	1477	SIA	3	0
5	A	1479	GOL	2	0
8	B	2485	MAN	1	0
4	D	4478	SIA	1	0
4	C	3478	SIA	2	0
5	C	3479	GOL	1	0
8	A	1486	MAN	1	0
4	A	1478	SIA	1	0
4	B	2477	SIA	1	0
6	A	1480	NAG	2	0
6	A	1481	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	3490	BMA	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SIA D 4477

Bond lengths

Bond angles

Torsions

Rings

Ligand SIA C 3477

Bond lengths

Bond angles

Torsions

Rings

Ligand SIA B 2478

Bond lengths

Bond angles

Torsions

Rings

Ligand SIA A 1477

Bond lengths

Bond angles

Torsions

Rings

Ligand SIA D 4478

Bond lengths

Bond angles

Torsions

Rings

Ligand SIA C 3478

Bond lengths

Bond angles

Torsions

Rings

Ligand SIA A 1478

Bond lengths

Bond angles

Torsions

Rings

Ligand SIA B 2477

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	389/389 (100%)	-0.39	1 (0%)	94	94	11, 17, 26, 41	0
1	B	389/389 (100%)	-0.36	3 (0%)	86	87	11, 17, 25, 48	0
1	C	389/389 (100%)	-0.44	3 (0%)	86	87	11, 17, 26, 41	0
1	D	389/389 (100%)	-0.37	1 (0%)	94	94	11, 17, 25, 38	0
All	All	1556/1556 (100%)	-0.39	8 (0%)	91	92	11, 17, 26, 48	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1089	THR	2.9
1	A	460	ARG	2.6
1	B	1088	ARG	2.4
1	D	3460	ARG	2.4
1	C	2088	ARG	2.3
1	C	2349	GLY	2.1
1	B	1094	THR	2.1
1	C	2460	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	G	1	14/15	0.49	0.33	35,40,42,43	0
2	NAG	E	1	14/15	0.57	0.35	54,62,63,64	0
2	NAG	F	1	14/15	0.63	0.30	35,39,40,41	0
2	NAG	E	2	14/15	0.63	0.36	40,44,47,47	0
3	BMA	G	2	11/12	0.69	0.27	63,67,69,71	0
2	NAG	H	2	14/15	0.71	0.31	33,38,43,47	0
2	NAG	H	1	14/15	0.72	0.38	41,43,45,46	0
2	NAG	F	2	14/15	0.73	0.35	29,40,42,43	0
3	MAN	G	3	11/12	0.79	0.23	51,54,57,59	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.
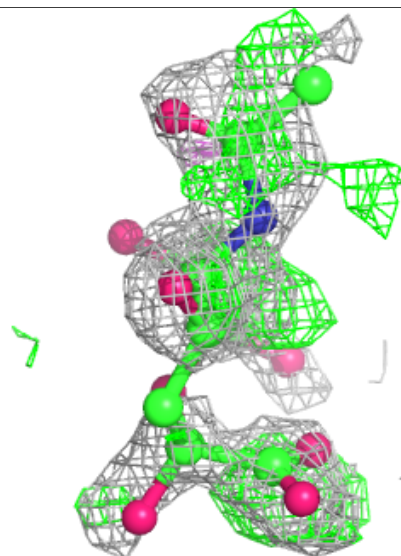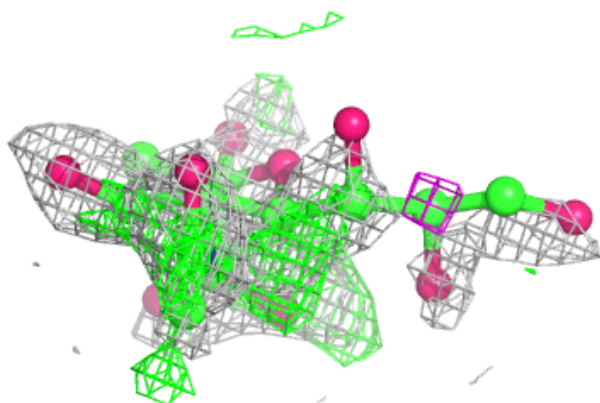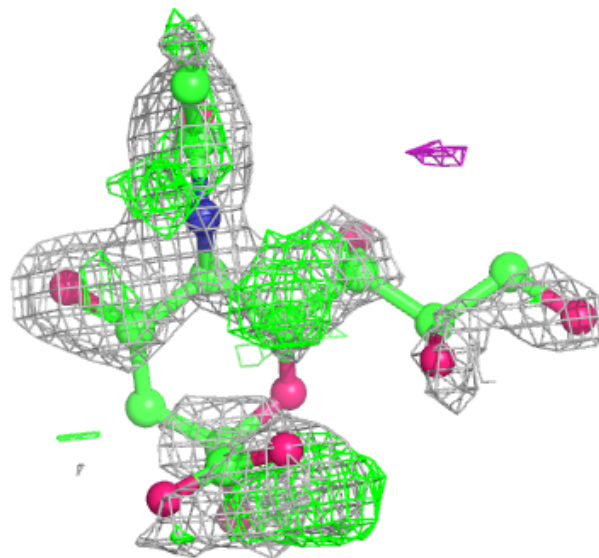

Electron density around Chain E:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
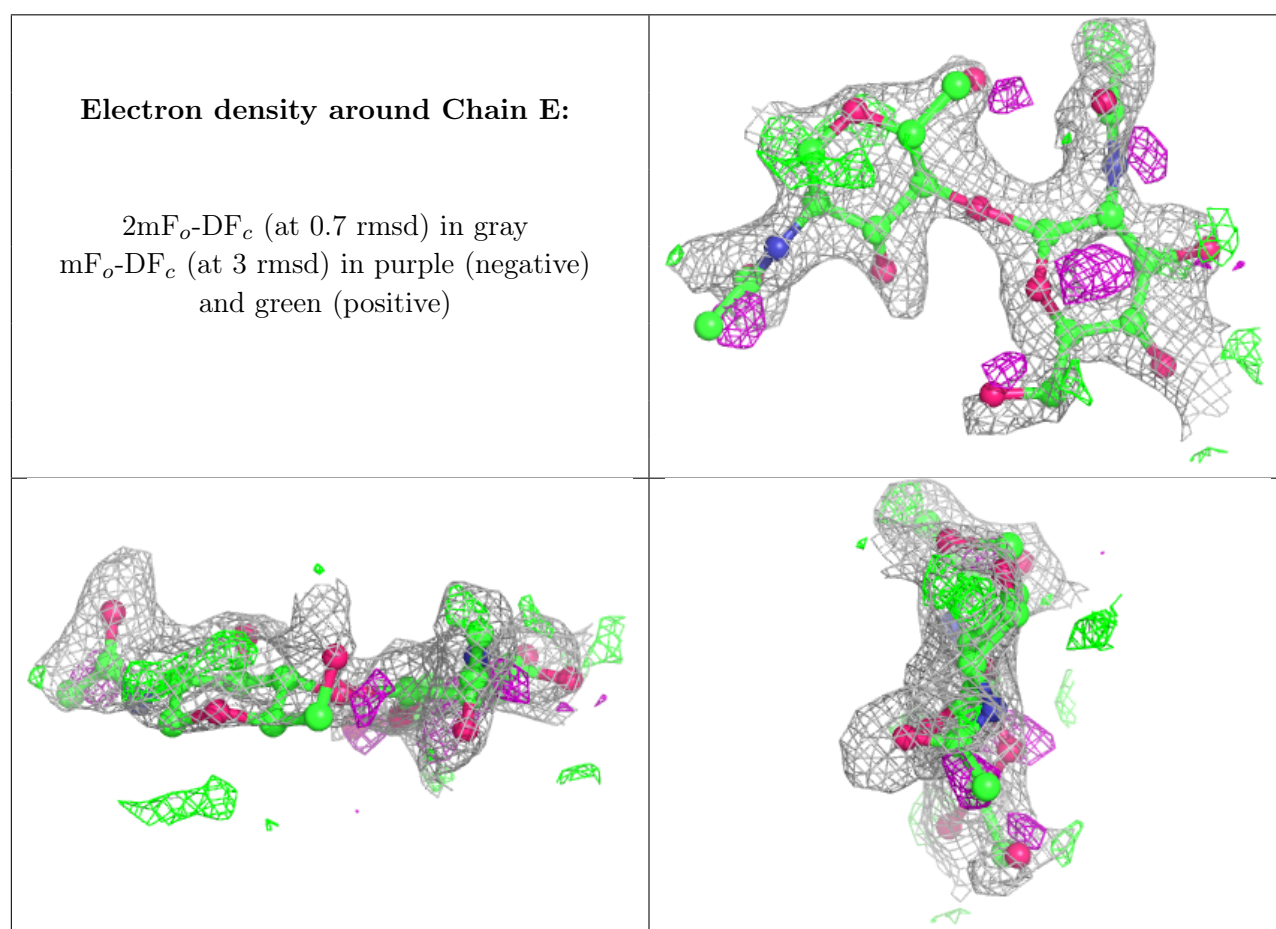
Electron density around Chain F:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
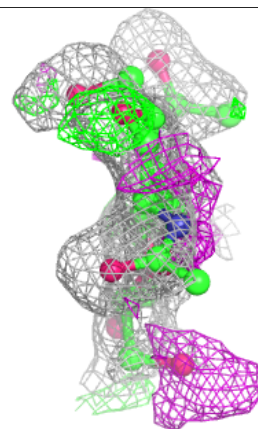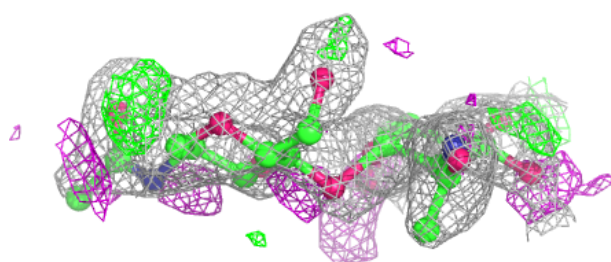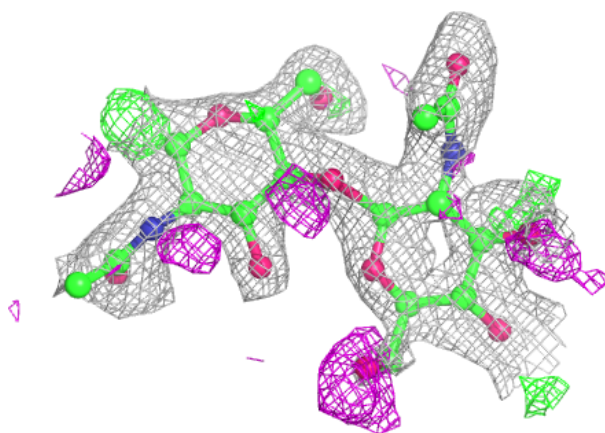
Electron density around Chain H:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
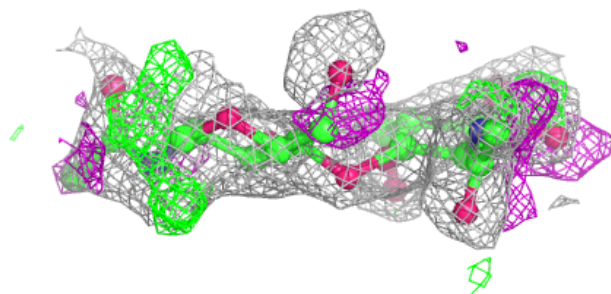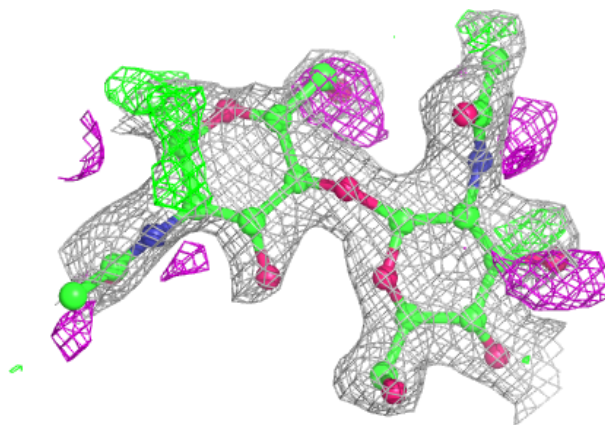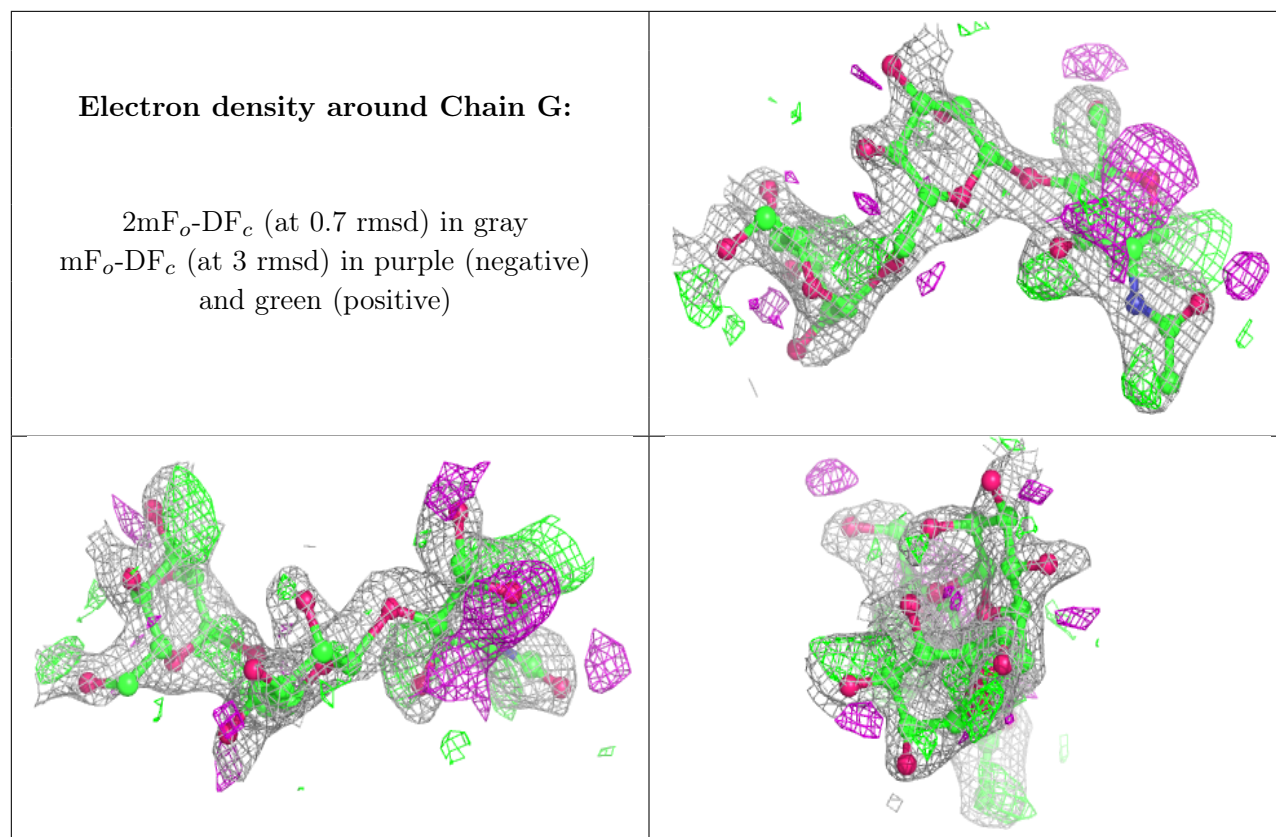
Electron density around Chain G:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	MAN	C	3486	11/12	0.42	0.52	95,96,96,97	0
4	SIA	C	3478	21/21	0.47	0.72	28,32,34,36	21
7	BMA	A	1484	11/12	0.56	0.34	57,62,69,69	0
8	MAN	A	1486	11/12	0.63	0.28	55,59,64,66	0
4	SIA	A	1478	21/21	0.63	0.46	16,19,22,23	21
8	MAN	B	2484	11/12	0.65	0.29	71,72,74,75	0
5	GOL	C	3479	6/6	0.65	0.24	25,30,32,33	0
5	GOL	B	2479	6/6	0.68	0.20	27,30,34,35	0
7	BMA	B	2483	11/12	0.69	0.40	61,68,72,72	0
8	MAN	A	1485	11/12	0.72	0.23	51,54,56,60	0
8	MAN	B	2486	11/12	0.72	0.35	67,73,75,76	0
4	SIA	D	4478	21/21	0.72	0.23	22,33,35,39	21
8	MAN	C	3485	11/12	0.74	0.28	60,61,64,69	0
8	MAN	B	2485	11/12	0.74	0.30	62,64,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
8	MAN	A	1487	11/12	0.75	0.22	41,52,54,60	0
5	GOL	A	1479	6/6	0.75	0.21	20,32,33,33	0
7	BMA	C	3490	11/12	0.76	0.28	58,64,65,66	0
6	NAG	D	4480	14/15	0.77	0.22	25,33,37,38	0
5	GOL	D	4479	6/6	0.78	0.21	24,34,36,37	0
8	MAN	C	3488	11/12	0.79	0.21	44,51,55,57	0
6	NAG	A	1480	14/15	0.80	0.23	36,42,44,45	0
4	SIA	B	2478	21/21	0.80	0.21	24,32,37,37	21
6	NAG	C	3481	14/15	0.81	0.18	27,30,34,37	0
8	MAN	C	3489	11/12	0.81	0.20	39,41,47,51	0
4	SIA	A	1477	21/21	0.84	0.16	17,19,23,24	0
6	NAG	B	2480	14/15	0.85	0.21	21,33,39,43	0
4	SIA	C	3477	21/21	0.85	0.17	16,19,22,24	0
4	SIA	B	2477	21/21	0.87	0.15	17,19,21,24	0
4	SIA	D	4477	21/21	0.87	0.15	17,20,23,27	0
6	NAG	A	1481	14/15	0.88	0.23	24,32,38,42	0
9	CA	A	1488	1/1	0.98	0.27	8,8,8,8	0
9	CA	B	2487	1/1	0.98	0.32	5,5,5,5	0
9	CA	C	3491	1/1	0.98	0.34	2,2,2,2	0
9	CA	D	4481	1/1	0.99	0.28	4,4,4,4	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
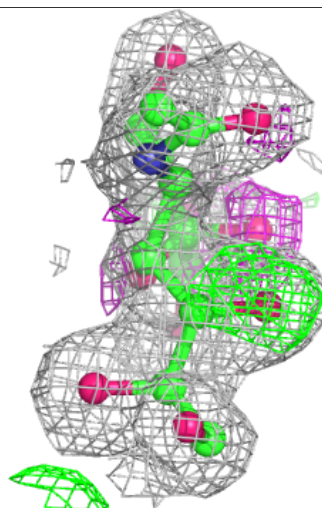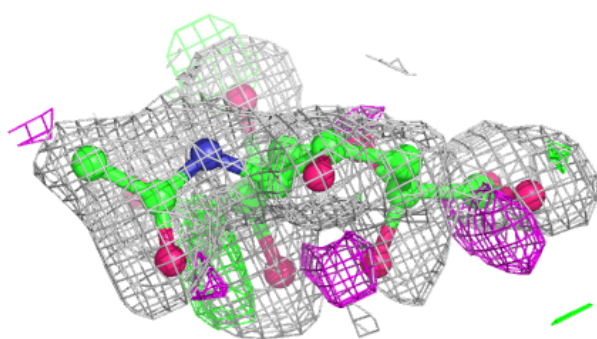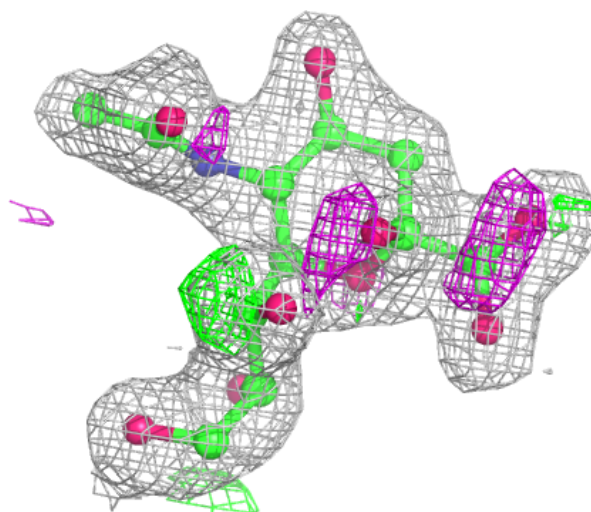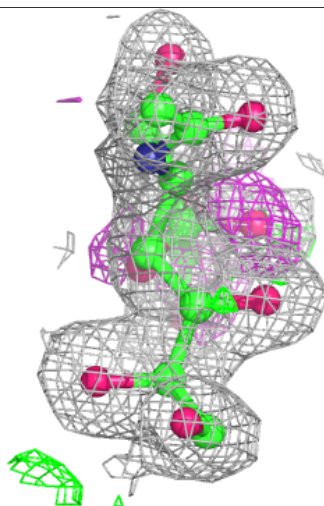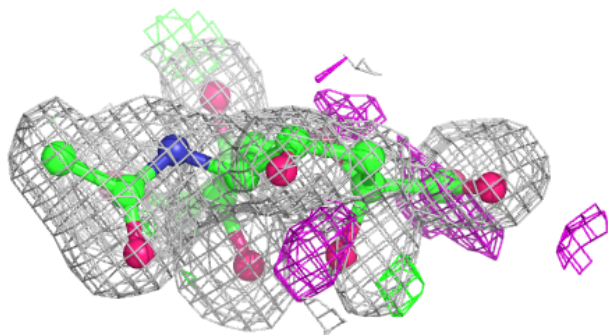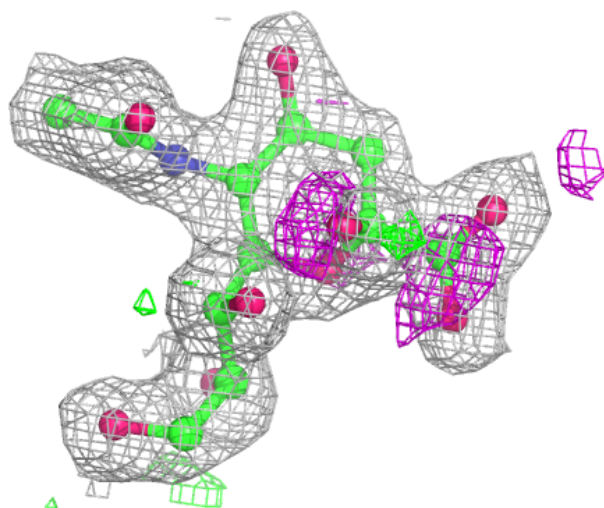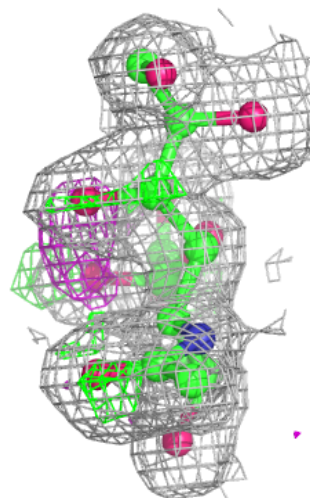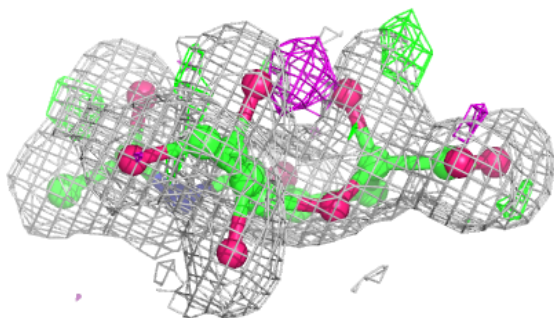
Electron density around SIA C 3478:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
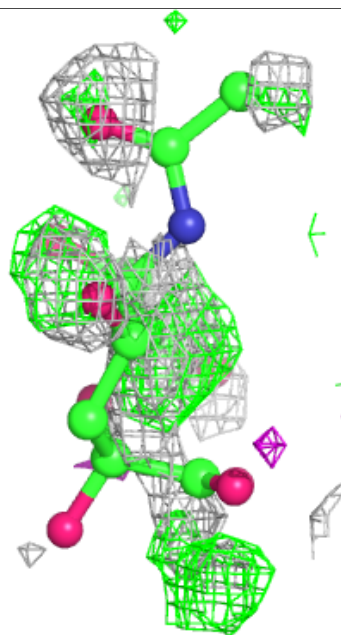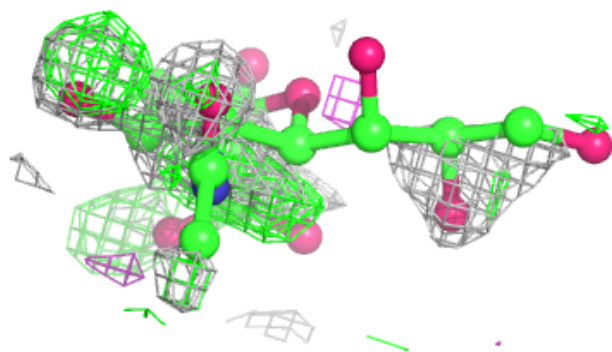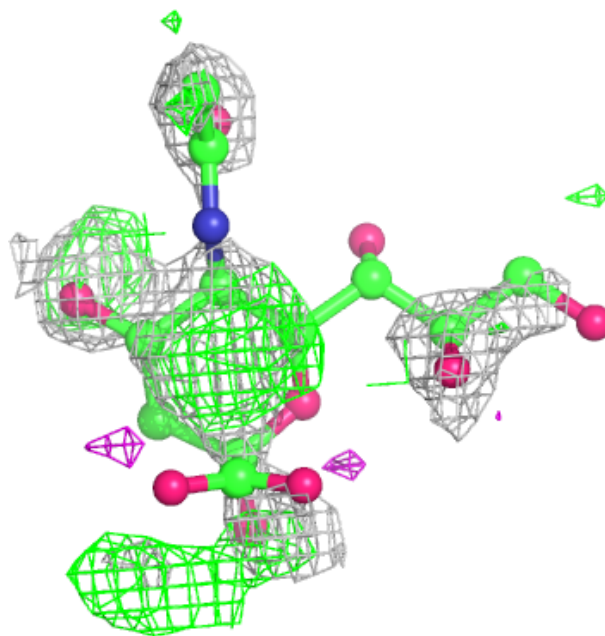
Electron density around SIA A 1478:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SIA D 4478:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
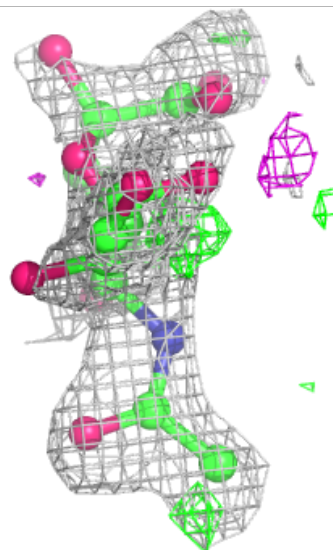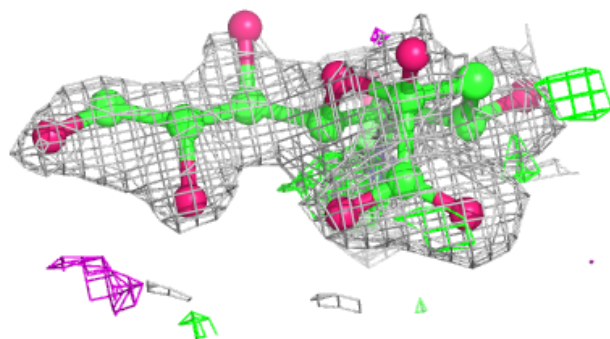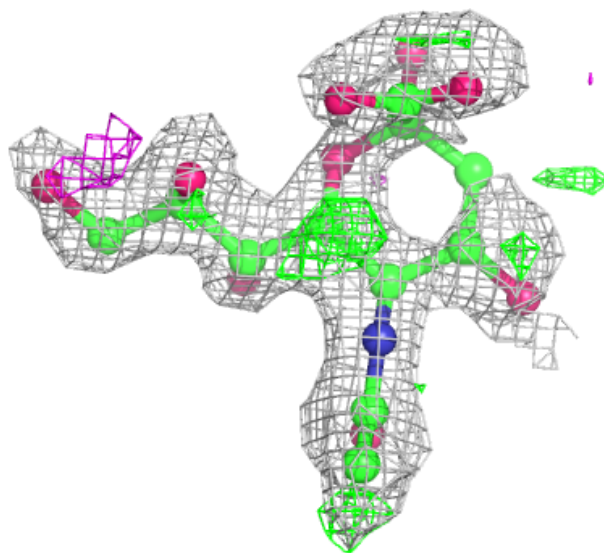
Electron density around SIA B 2478:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
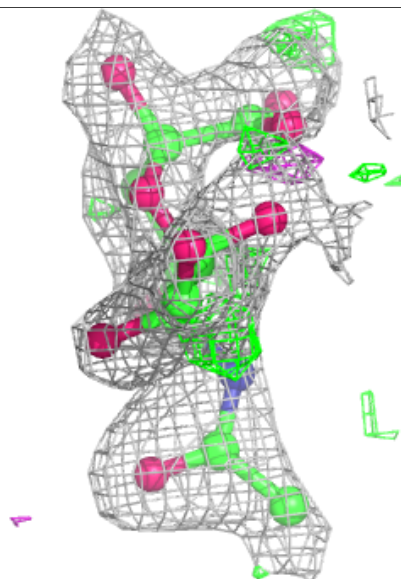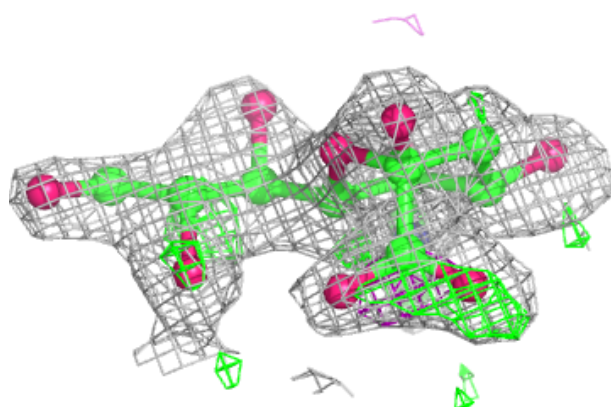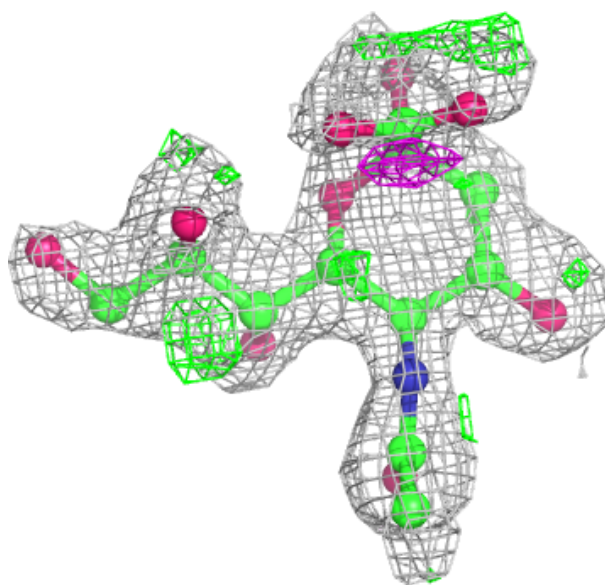
Electron density around SIA A 1477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
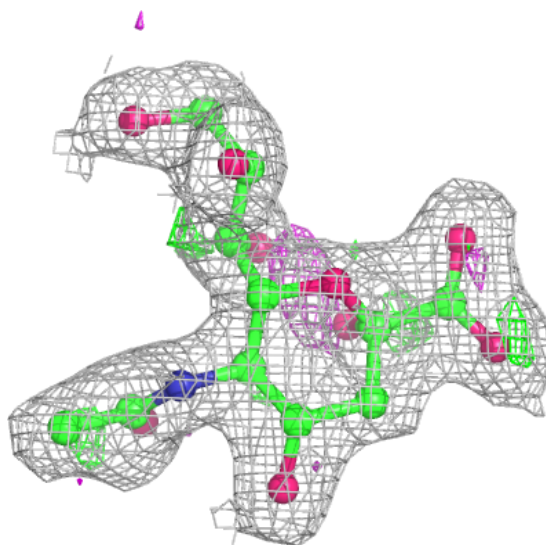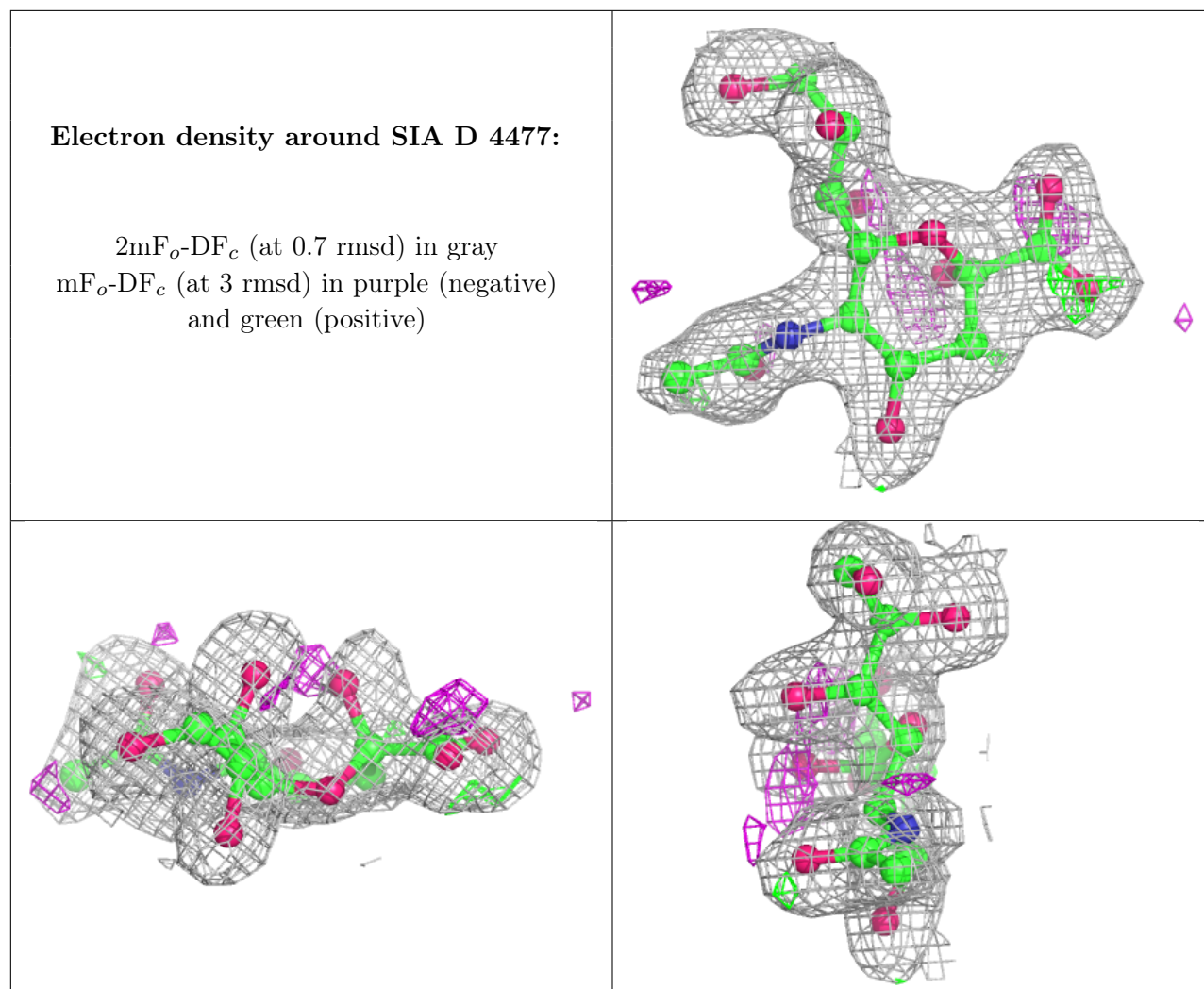and green (positive)

Electron density around SIA C 3477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SIA B 2477:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SIA D 4477:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.